### **ENGINEERING OF CHEMICAL COMPLEXITY**

11<sup>th</sup> International Conference July 29 – August 1, 2025, Tokyo, Japan.







### **Tuesday, July 29, 2025**

	I			
8:15 am	Registration			
8:45 am	Opening and Welc	ome		
9:00 am	Emergent Order and Non-Reciprocal			
Plenary	I. Pagonabarraga Interactions in Active Matter: From			
talk		Synchronization to Phase Separation		
	R. Yamamoto,			
1	Active matter and	collective dynamics	J. Simmchen	
10:00 am	S. Schnyder	Epidemics with Altrui	ism	
10.30 am	K. Henze	Broadening fuel options for spherical Janus microswimmer and their impact on the swimming behavior		
11:00 am	Coffee Break/Discussion			
11:30 am	S. Tanaka	Droplet robots composed of self-propelled droplets on the surface of aqueous solutions		
11:45 am	N. Suematsu Synchronization of Chemical Oscillatory			
		Reaction in Active Dr	•	
12:00 pm	A. Gamez	Collective Motion in I Synchronisation and I		
12:15 pm	H. Noguchi		rns in active Potts models	
12:30 pm	Lunch			
	Open topics			
2:00 pm	J. Simmchen		terial have to be to mimic	
		biological behaviours		
2:15 pm	H. Kitahata	Diffusiophoretic Motion coupled with Droplet Shape		
2:30 pm	I. Azizi	Active Fluids with Long-Range Interactions		
2:45 pm	I. Kawamata	Engineering DNA Chemical Reaction Network for Autonomous Assembly and Disassembly of Active Matter		
3:00 pm	Y. Kato	Bayesian comparison of Langevin models from single tracking datasets of cell motility		
3:15 pm	T. Sukegawa	Numerical Analysis for Synchronization Tran Mechanical Oscillation	or Controlling sition of Chemo-	

3:30 pm	T. de Jong	de Jong  Harnessing any Kuramoto-like oscillator network as computational resource		
3:45 pm	L. Negrojevic	Adaptive maze solving by frozen fronts		
4 pm	Coffee Break/Discussion			
2	Cell motility and	microswimmers	C. Beta, H. Stark	
4:30 pm	A. Lindner	From individual trajectin suspensions of E-co	tories to collective motion li bacteria	
5:00 pm	S. Karpitschka		to Collective Swimming: ilamentous Cyanobacteria	
5:30 pm	R. Großmann	Deciphering the motility pattern and dual chemotaxis strategy of bacteria in porous media		
5:45 pm	B. Nakayama	Fluctuation-driven Propulsion in a Self- produced Viscosity Gradient		
6:00 pm	H. Stark	Modeling microorganisms: Escherichia coli and Trypanosoma brucei		

### Wednesday, July 30, 2025

	Chemical/biologic	al information	T. Kobayashi,	
6	processing		D. Loutchko	
9:00 am	T. Kobayashi	Controlling Biological Reaction Networks		
9:30 am	M. Liero  Generalized gradient sy thermodynamically con including temperature of		nsistent modeling	
10:00 am	S. Toyabe	Kinetic proofreading a replication inherited in	_	
10:30 am	G. Rotskoff	Designing Nonequilibrates Reinforcement Learning	rium Assemblies with ng and Optimal Transport	
11:00 am	Coffee Break/Disci	ussion		
11:30 am	<b>Poster Session</b>			
12:30 pm	Lunch			
7	Fluctuations and r	nano-scale dynamics	K. Takeuchi, H. Flechsig	
2:00 pm	S. Tani	Dynamics of surface morphology driven by ultrashort laser pulses		
2:30 pm	N. Akutsu	Partial Breakdown of the Kolmogorov-Johnson- Mehl-Avrami Theory in a Two-Dimensional Poly-Nuclear Process on the Kardar-Parisi- Zhang Kinetic Rough (001) Surface During Steady Crystal Growth		
2:45 pm	E. Tjhung	Exact Results in Stock Division, Death, and L		
3:00 pm	M. Shibata		ng of 12meric CaMKII	
3:30 pm	S. Shinkai	Fluctuation of the 3D Genome from Modeling and Experiments		
4:00 pm	Coffee Break/Disco	ussion		
4:30 pm Plenary talk	A. E. Motter	Converse Symmetry Bi	reaking	
5:30 pm	Get-together with discussions, sr	nacks and finger food		

### Thursday, July 31, 2025

5	Pattern formation organization	and biological self-	M. Falcke, H. Kitahata	
9:00 am	M. Sano		collective behavior around bottom-up approach to umics	
9:30 am	T. Nakagaki	Behavioral Patterns of Protists in Relatively Complex Experimental Environments		
10:00 am	M. Eberhard	The universal speed-persistence relation of cells moving on 1D fibronectin lanes is biphasic		
10:15 am	A. Gholami	Curved Boundaries Da Rotational Motion in A		
10:30 am	K. Takeuchi	Smectic-like bundle fo bacteria upon nutrient	0 1	
10:45 am	R. Muolo	Theory of Turing patterns on discrete topologies: from networks to hypergraphs		
11:00 am	Coffee Break/Disc	ussion		
11:30 am	<b>Poster Session</b>			
12:30 pm	Lunch			
			I 7 IZ IZ IZ I	
4	Oscillation and sy	nchronization	I. Z. Kiss, K. Krischer, H. Kori	
2:00 pm	Oscillation and sy  A. Yochelis	Rogue-like Waves in a	H. Kori	
		Rogue-like Waves in a System: Stochastic Ou Dynamics Si Electrodissolution o	H. Kori  Reaction-Diffusion  tput from Deterministic	
2:00 pm	A. Yochelis	Rogue-like Waves in a System: Stochastic Ou Dynamics Si Electrodissolution of Collective Oscillatory Experiment Understanding and Collections in Reaction-like	H. Kori  Reaction-Diffusion  tput from Deterministic  as a Model System for Behavior: Theory and  ontrolling Oscillatory	
2:00 pm 2:30 pm	A. Yochelis Y. Murakami	Rogue-like Waves in a System: Stochastic Ou Dynamics Si Electrodissolution of Collective Oscillatory Experiment Understanding and Collection in Reaction-Labely by Developing in	H. Kori Reaction-Diffusion Atput from Deterministic  The sa Model System for Behavior: Theory and  Controlling Oscillatory Diffusion Systems with Phase Reduction Method  The ted to pattern formation on	
2:00 pm 2:30 pm 2:45 pm	A. Yochelis  Y. Murakami  A. Ozawa	Rogue-like Waves in a System: Stochastic Ou Dynamics Si Electrodissolution of Collective Oscillatory Experiment Understanding and Collective Patterns in Reaction-Landing by Developing Inverse problems relationally coupled oscillator net	H. Kori Reaction-Diffusion Atput from Deterministic  The sa Model System for Behavior: Theory and  Controlling Oscillatory Diffusion Systems with Phase Reduction Method  ted to pattern formation on works equencies in slime mold	
2:00 pm 2:30 pm 2:45 pm 3:00 pm	A. Yochelis  Y. Murakami  A. Ozawa  O. Omel'chenko	Rogue-like Waves in a System: Stochastic Ou Dynamics Si Electrodissolution of Collective Oscillatory Experiment Understanding and Conference of Patterns in Reaction-lay by Developing Inverse problems related to the Coupled oscillator network Multiple oscillation from transportation network chimera states Bistability between systems	H. Kori Reaction-Diffusion Atput from Deterministic  The sa Model System for Behavior: Theory and  Controlling Oscillatory Diffusion Systems with Phase Reduction Method  ted to pattern formation on works equencies in slime mold	

4:20 pm Special talk	Y. Kuramoto	Some recollections from my past works		
5:30 pm	Conference dinner (details will be announced later)			

### Friday, August 1, 2025

	I				
3	Control and design of self-organization		J-S. Li, H. Nakao,		
		R. Muolo			
9:00 am	V. Narayanan		Curvature Analysis for Inferring Nonlinear Dynamics: Applications in Reconstructing		
9:30 am	A. Bigaj	Instabilities of a bimolecular reaction driven by buoyant flows			
9:45 am	H. Ninomiya		Turing instability in reaction-diffusion systems with equal diffusion coefficients		
10:15 am	K. Krischer	Hierarchies of Cluster S Coupled Oscillators	Hierarchies of Cluster States in Ensembles of		
10:30 am	D. Proverbio	, ,	Self-organization of optimal network formation: emerging capabilities of Physarum polycephalum		
11:00 am	Coffee Break/Dis	cussion			
	Open topics				
11:30 am	Y. Ye	Optically and Electrical Colloids in Liquid Crys (Invited talk of Symposi	tals		
12:00 pm	N. Namura	Numerical simulations of hexapod gait patterns by a CPG network composed of oscillatory chemical systems			
12:15 pm	Y. Mitsui	Synchronization-induced Taylor's law in coupled periodic and chaotic oscillators			
12:30 pm	Lunch				
2:00 pm	M. Tarama	Synchronization mechan control	nism of elevators and its		
2:15 pm	A. Matsuki	Network inference from signals based on the cir	synchronous oscillatory cle map		
2:30 pm	M. Falcke	Spike generation as firs Stochastic model of IP3 of HEK293 cells			
2:45 pm	S. Guido	The effect of mechanica formation in cell sphero	-		
3:00 pm Plenary talk	A. De Wit	Self-organised patterns advection systems	in reaction-diffusion-		
4:00 pm	Closing remarks				

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Y. Kuramoto		nary talk pecial tall		Fri Thu	3 1
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K. Henze	and collective	2	Invited talk	Tue	6
S. Tanaka	dynamics	3	Contributed talk	Tue	7
N. Suematsu	<i>a.j.</i> 1	4	Contributed talk	Tue	8
A. Gamez		5	Contributed talk	Tue	9
H. Noguchi		6	Contributed talk	Tue	10
A. Lindner	2 - Cell motility	15	Invited talk	Tue	11
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# **Emergent Order and Non-Reciprocal Interactions in Active Matter: FromSynchronization to Phase Separation**

### Ignacio Pagonabarraga

Department of Fundamental Physics at the University of Barcelona

Active matter consists of self-driven units that continuously dissipate energy to generate motion and internal stresses, giving rise to rich collective behavior far from equilibrium. Capturing this behavior requires a physicochemical framework that integrates self-propulsion, alignment interactions, and the coupled transport of momentum, orientation, and density.

I will present minimal models of aligning active particles inspired by Kuramoto-type interactions. These systems exhibit orientational ordering and reveal how activity modifies classical transitions such as the Kosterlitz-Thouless transition. In particular, I will show that motility can stabilize long-range order in systems with XY symmetry and qualitatively alter the dynamics of topological defects, leading to broken reciprocity and long-range correlations. I will also explore how passive inclusions embedded in an active fluid interact through stress-mediated, non-reciprocal forces and influence the global organization of the medium. Altogether, these results uncover key mechanisms by which self-propulsion, alignment, and dynamic symmetry breaking govern emergent structure and phase behavior in active materials.

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### **Converse Symmetry Breaking**

#### Adilson E. Motter

Center for Network Dynamics and Department of Physics & Astronomy Northwestern University, Evanston, Illinois, USA

Symmetry breaking, where a system's symmetry is not inherited by its stable states, drives numerous effects in physics. This talk will discuss converse symmetry breaking, a striking emergent phenomenon where stable states can be symmetric only when the system itself is not. Through theoretical predictions and experimental demonstrations, I will illustrate its relevance and applications to diverse network problems. Additionally, I will discuss how this phenomenon challenges conventional assumptions, revealing that behavioral homogeneity often necessitates underlying system heterogeneities. Ultimately, I hope to convey that our study of network systems not only builds on statistical and nonlinear physics but also contributes to foundational discoveries in these fields.

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### Self-organised patterns in reaction-diffusion-advection **systems**

#### **Anne De Wit**

Nonlinear Physical Chemistry Unit, Université libre de Bruxelles, Brussels, Belgium

The interplay between autocatalytic reactions and diffusion can lead to selforganised reaction-diffusion (RD) patterns such as traveling fronts, waves, and Turing patterns. In my talk, I will review how injection of a solution of one reactant of such systems into another reactant can produce new patterns.

Specifically, the presence of radial advection will be shown both theoretically and experimentally to be able to freeze autocatalytic fronts at a given radius when the reactant is injected into a solution of the autocatalyst [1]. In presence of a diffusive instability of such RD fronts, these frozen fronts can evolve into sun-like shaped structures [2].

In the case of a precipitation reaction, the presence of radial advection can induce the self-organisation of the precipitate along phyllotactic patterns [3], similar to those observed in botany [4] or dynamical physical systems [5]. I will discuss how radial advection can also influence Turing patterns [3].

Eventually, I will address the case of saddle flows and show how they can force traveling waves to self-organise into wave packets [6].

These various examples will evidence how flows can interplay with the selforganising power of nonlinear chemical systems to produce new spatiotemporal dynamics.

- 1. L. Negrojević, A. Comolli, F. Brau, A. De Wit, Phys. Rev. Research 6, L042044 (2024).
- 2. S. Maharana, L. Negrojevic, A. Comolli, A. De Wit, submitted.
- 3. G. Facchini, M. Budroni, G. Schuszter, F. Brau, A. De Wit, submitted.
- 4. R.V. Jean, Phyllotaxis: A Systemic Study in Plant Morphogenesis (Cambridge University Press, Cambridge, 1994).
- 5. S. Douady, Y. Couder, Phys. Rev. Lett. 68, 2098 (1992).
- 6. S. Izumoto, D.M. Escala, J. Heyman, T. Le Borgne, A. De Wit, Phys. Rev. Lett., 133, 218001 (2024).

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### Some recollections from my past works

### Yoshiki Kuramoto

Department of Physics, Kyoto University

Regarding some of the works I accomplished in the past, anecdotal stories on how they came to fruition will be presented.

### Symposium 1: Active matter and collective dynamics

### Ryoichi Yamamoto, Juliane Simmchen

#### Epidemics with Altruism

Mark P. Lynch <sup>1</sup>, <u>Simon K. Schnyder</u> <sup>2</sup>, John J. Molina <sup>3</sup>, Ryoichi Yamamoto <sup>3</sup>, Matthew S. Turner <sup>4,5</sup>

Behaviour affects the spread of infectious diseases. Earlier, we studied self-organised social distancing among purely self-interested individuals during an epidemic using game theory [1]. There, we leveraged an analytic solution for behaviour and corresponding disease dynamics to derive a simple relationship between rational social distancing behaviour and the current number of infections as well as the cost of infection. While higher infection costs lead to stronger social distancing, a population of completely self-interested individuals would not tend to social distance strongly enough to avoid herd immunity.

The quarantining of infected individuals can significantly reduce the spread of most diseases but epidemiologists typically assume that such quarantining requires external enforcement, e.g. by government. However, individuals likely possess at least some degree of altruism and may be motivated to protect others by voluntarily self-quarantining when infected. Despite this possibility, research on how altruism influences individual behaviour during epidemics remains limited.

Here, we demonstrate that even extremely weakly altruistic individuals, who prioritise their own interests far above those of others, may spontaneously choose to self-quarantine when infected. This voluntary behaviour can reduce disease transmission strongly enough to avoid herd immunity through infection. The disease suppression via self-quarantine can remain effective despite moderate rates of asymptomatic cases or the presence of entirely self-interested individuals. Although our findings derive from complex optimisation calculations, the observed behaviour could have developed as a straightforward evolutionary strategy.

1. S. K. Schnyder, J. J. Molina, R. Yamamoto, and Matthew S. Turner, PNAS  $\mathbf{122}$ , e2409362122 (2025).

<sup>&</sup>lt;sup>1</sup>Mathematics of Systems CDT, University of Warwick, Coventry, UK.

<sup>&</sup>lt;sup>2</sup>Institute of Industrial Science, The University of Tokyo, Tokyo, Japan.

<sup>&</sup>lt;sup>3</sup>Department of Chemical Engineering, Kyoto University, Kyoto, Japan.

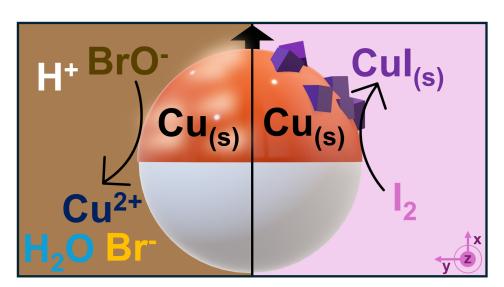
<sup>&</sup>lt;sup>4</sup>Department of Physics, University of Warwick, Coventry, UK.

<sup>&</sup>lt;sup>5</sup>Institute for Global Pandemic Planning, University of Warwick, Coventry, UK.

### Broadening fuel options for spherical Janus microswimmer and their impact on the swimming behavior

 $Kelly\ Henze\ ^1,\ Zuyao\ Xiao\ ^1,\ Khalifa\ Mohamed\ ^2,\ Juliane\ Simmchen\ ^2$ 

Janus particles play an essential role in the field of active matter, particularly as microswimmers. The most popular propulsion mechanism relies on the catalytic decomposition of hydrogen peroxide. However, expanding the range of available fuels is essential for enhancing biocompatibility, reducing toxicity, and improving efficiency, especially for environmental and medical applications. This talk will focus on halogen-based propulsion mechanisms in Janus microswimmers, focusing on a redox-driven approach using bromine and iodine as fuel sources. [1,2] By analyzing the swimming behavior of spherical Cu@SiO2 microswimmers, we compare their motion to the highly studied hydrogen peroxide-driven systems. Our findings reveal distinct differences in propulsion efficiency and velocity trends, highlighting the influence of redox product solubility on microswimmer dynamics. Furthermore, the talk will show a fundamental reorientation effect after the microswimmer activation with the different fuels, revealing a fundamental influence across the broad of microswimmer systems. [3] By investigating alternative fuels and their impact on microswimmer behavior, we contribute to the development of new application fields and a deeper understanding of active particle dynamics.



- 1. K. Henze, Z. Xiao et al., Chem. Commun., (2025).
- 2. R. Liu, A. Sen, J. Am. Chem. Soc., (2025). 133, 50, (2011).
- 3. J. Simmchen, J. Katuri et al., Nat. Commun., 7, 10598 (2016).

<sup>&</sup>lt;sup>1</sup>Freigeist group, Physical Chemistry TU Dresden, Zellescher Weg 19, 01062 Dresden, DE

<sup>&</sup>lt;sup>2</sup>Pure and Applied Chemistry, University of Strathclyde, Glasgow G1 1BX, UK

### Droplet robots composed of self-propelled droplets on the surface of aqueous solutions

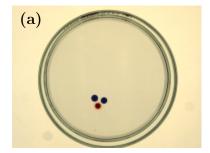
Shinpei Tanaka <sup>1</sup>, Rony Mallick <sup>1</sup>, Chiho Watanabe <sup>2</sup>

It is well-known that active particles exhibit variety of motion patterns, including intermittent oscillation, orbitting motion, or predator-prey chasing [1]. One of the next steps in this research field is to create functions out of motion patterns of active particles. In this presentation, we show the possibility to design robot composed of macroscopic droplets self-propelled on the surface of aqueous solutions [2].

Figure 1 shows examples of our droplet robots. Blue droplets in the figure are composite droplets made of 1-decanol and polydimethylsiloxane (PDMS). Dissolution of 1-decanol molecules changes the surrounding surface tension. PDMS controls the dissolution rate to give the robots stability. Red droplets are made of ethylsalicylate (ES), which absorb 1-decanol. These droplets generate an inhomogeneous surface tension field around them, driving their motion.

Interestingly, we found that the configuration of droplets determines their functions. When a robot has a front-back asymmetry, that is, it has a head in which direction it moves as shown in Fig. 1(a), the motion pattern becomes rather linear. On the other hand, when a robot does not have such broken symmetry as shown in Fig. 1(b), it moves randomly. The broken symmetry can be built-in in the configuration of a robot, or it appears as a result of self-propulsion.

By analogy to biology, the robot shown in Fig. 1(a) can be considered a bilaterian, well-suited for directed movement toward a target. The robot shown in Fig. 1(b), on the other hand, is a radiata, which excels in search and exploration. Therefore, their functions arise from their respective body plans. In the presentation, we aim to demonstrate and discuss the design of droplet robots and the realization of their functions in a broader context.



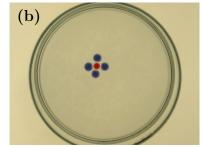


Figure 1: Droplet robots. (a) Two active droplets (blue) push a passive one (red). The cluster exhibits back-and-forth motion. (b) Four active droplets encircle a passive one. They move randomly together.

- 1. C. Watanabe, S. Tanaka, R. J. G. Löffler, M. M. Hanczyc and J. Górecki, *Soft Matter*, **18**, 6465-6474, (2022)
- 2. R. Mallick, C. Watanabe, and S. Tanaka, Phys. Chem. Chem. Phys., accepted.

<sup>&</sup>lt;sup>1</sup>Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima, Japan.

<sup>&</sup>lt;sup>2</sup>Graduate School of Integrated Sciences for life, Hiroshima University, Higashi-Hiroshima, Japan.

### Synchronization of Chemical Oscillatory Reaction in Active Droplets

<u>Nobuhiko</u> J. Suematsu <sup>1,2</sup>

<sup>1</sup>Graduate School of Advanced Mathematical Sciences, Meiji University, Tokyo, Japan <sup>2</sup>Meiji Institute for Advanced Study of Mathematical Sciences (MIMS), Meiji University, Tokyo, Japan

Synchronization of oscillators is a phenomenon commonly observed in nature. In biological systems, synchronization creates essential functionalities; for instance, the beating heart relies on the synchronized oscillations of nearby cells. Similar behaviors are found in chemical oscillatory reactions. One well-known example is the Belousov-Zhabotinsky (BZ) reaction, where the synchronization of oscillations can be easily seen in reactions occurring within beads or droplets [1]. The distance between these beads or droplets typically influences the coupling strength. Therefore, when the droplets move spontaneously and exhibit collective motion, the coupling strength can change dynamically over time.

Recently, self-propelled aqueous droplets have been reported to move within an oil phase containing surfactants [2]. In our study, we demonstrated self-propelled BZ droplets and observed the synchronization of the chemical oscillators. The droplets spontaneously formed clusters, leading to in-phase synchronization within these clusters. These behaviors can be explained by the attractive coupling mediated by the activator  $\mathrm{HBrO}_2$  [1]. In contrast, the repulsive interaction through  $\mathrm{Br}_2$  appears negligible due to the interfacial chemical reaction with the surfactant, which generates a driving force for the self-propelled motion.

Our system provides a straightforward experimental platform for the swarmalator model [3, 4] and could eventually allow the reproducibility of swarmalator behavior in real-world systems.

- 1. M. M. Norton, N. Tompkins, B. Blanc, M. C. Cambria, J. Held, and S. Fraden, *Phys. Rev. Lett.* **123**, 148301 (2019).
- 2. N. J. Suematsu, Y. Mori, T. Amemiya, and S. Nakata, *J. Phys. Chem. Lett.* **12**, 7526 (2021).
- 3. D. Tanaka, *Phys. Rev. Lett.* **99**, 134103 (2007).
- 4. G. K. Sar and D. Ghosh, Europhys. Lett. 139, 53001 (2022).

#### Collective Motion in Microswimmers: Synchronisation and Flocking

Antonio J. Gamez<sup>1</sup>, Hiroshi Kori<sup>2</sup>

The collective motion of microswimmers, such as bacteria, active colloids, and motile cells, emerges from their local interactions and self-propulsion [1]. These systems exhibit rich dynamical behaviours, including clustering, swarming, and spontaneous pattern formation, often governed solely by hydrodynamic interactions [2, 3]. Understanding the fundamental mechanisms behind these emergent phenomena is essential for both theoretical modelling and practical applications. However, active matter models are typically complex, and simulations can be computationally expensive, even for a small number of individuals [4]. Furthermore, few models in the literature simultaneously address synchronisation and flocking, and most are phenomenological in nature [5].

In this work, we propose a simple yet realistic model of microswimmers characterised by two intrinsic variables in addition to their position and velocity: their natural swimming frequency and alignment. By systematically varying these parameters, we explore the emergence of different collective states, such as synchronisation and flocking, and identify the conditions under which they arise [6, 7]. We analyse how these behaviours depend on the key parameters of the system and discuss their implications for understanding self-organisation in active matter. Finally, we outline possible directions for extending this model to incorporate external hydrodynamic interactions [8].

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#### Spatiotemporal patterns in active Potts models

Hiroshi Noguchi

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We studied the effects of thermal fluctuations using MC simulations of active Potts models with three [1-3] or four states [4]. It is a model system for chemical reactions on a catalytic surface or molecular transport through a membrane.

In a cyclically symmetric condition of three states, the homogeneous dominant states cyclically change via nucleation and growth at low cycling energy. In contrast, spiral waves are formed at high energy. The waves are generated from the contacts of three states. In medium cycling energies, these two modes temporally coexist. This transition can be understood from the competition between nucleation and growth of different states [1]. Biphasic domains can ballistically move in asymmetric conditions [2,3]. For the Potts model of four states, the spatial coexistence of two diagonal phases also occurs [4].

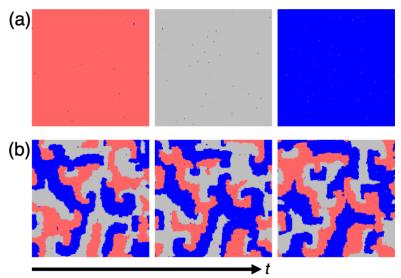


Fig. 1: sequential snapshots of three-state Potts model [1]. (a) Homogeneous cycling mode at low cycling energy. (b) Spiral wave mode at high cycling energy.

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### Symposium 2: Active matter and collective dynamics

### Carsten Beta, Holger Stark

#### From individual trajectories to collective motion in suspensions of E-coli bacteria Anke Lindner<sup>1</sup>

<sup>1</sup>PMMH-ESPCI, Paris, France

Active fluids consist of self-propelled particles (as bacteria or artificial microswimmers) and display properties that differ strongly from their passive counterparts. Unique physical phenomena, as enhanced Brownian diffusivity, viscosity reduction, active transport and mixing or the extraction of work from chaotic motion, result from the activity of the particles, locally injecting energy into the system. The presence of living and cooperative species may also induce collective motion and organization at the mesoscopic or macroscopic level impacting the constitutive relationships in the semi-dilute or dense regimes.

Individual bacteria transported in viscous flows show complex interactions with flows and bounding surfaces resulting from their complex shape as well as their activity. Understanding these transport dynamics is crucial, as they impact soil contamination, transport in biological conducts or catheters, and constitute thus a serious health thread. Here we investigate the trajectories of individual E-coli bacteria in confined and complex geometries with and without flow, using microfluidic model systems in combination with a novel Langrangian 3D tracking method. Combining experimental observations and modelling we elucidate the origin of upstream swimming, lateral drift, persistent transport along edges as well as bacteria accumulation in specific geometries.

Increasing bacteria concentrations collective motion emerges, where typical lengthscales can be identified in the velocity correlations. Using PIV measurements, we characterize the emerging vortex like structures as a function of confinement and we discuss how the corresponding lengthscale can be controlled though bounding walls or flows.

The understanding gained can be, for example, used to control bacteria transport in complex geometries or shed light on the role of emergent mescoscopic structures on the macroscopic properties of active suspensions.

## From Gliding Motility to Collective Swimming: The Many Talents of Filamentous Cyanobacteria

Maximilian Kurjahn <sup>1</sup>, Antaran Deka <sup>1</sup>, Franziska Papenfuß <sup>1</sup>, <u>Stefan Karpitschka <sup>1,2</sup></u>

Filamentous cyanobacteria are one of the oldest and today still most abundant lifeforms on Earth, with manifold implications in ecology and economics. Individual filaments are flexible, often several hundred cells long, and exhibit longitudinal gliding motility in contact with solid surfaces or other filaments. The direction of motion is subject to reversals which may be induced by various stimuli, most notably light gradients. The combination of large shape anisotropy, motility, and responsive behavior enables ensembles of filaments to contract into macroscopic, highly entangled colonies which perform collective motion and respond to environmental conditions. It is generally believed that their evolutionary success arises from these traits [1], but neither the physical mechanism behind gliding motility, nor the principles of their active aggregation and self-organization are currently understood. In this talk I will present our current research on this system, starting from a quantification of the gliding forces by analyzing self-buckling instabilities of individual filaments [2]. This enables quantitative simulations of ensembles of filaments [3], subject to stochastic and responsive reversals. Comparing simulations to experimental results on aggregation and alignment in response to illumination patterns [4], we elucidate principles that enable the bacteria to perform collective mechanical actions and govern the morphogenesis of cyanobacterial colonies.

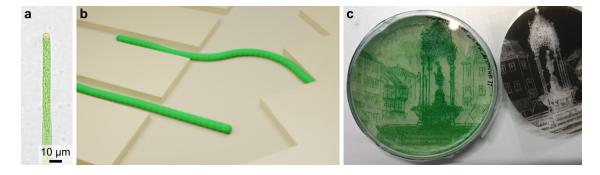


Figure 1: Filamentous Cyanobacteria: From individual filaments to collective self-organization. **a**, Small part of a filament of the species *Kamptonema animale*. **b**, Self-buckling instabilities of filaments gliding onto obstacles can be used to quantify gliding forces. **c**, "Cyanograph": Filaments preferentially populate bright regions, the superimposed, self-organized aggregation leaves the impression of a brush stroke.

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## Deciphering the motility pattern and dual chemotaxis strategy of bacteria in porous media

R. Großmann<sup>1</sup>, A. Datta<sup>1</sup>, S. Beier<sup>1</sup>, V. Pfeifer<sup>1</sup> and C. Beta<sup>1,2</sup>

Understanding the fundamental principles governing bacterial motility and navigation is key to comprehend important phenomena, such as infectious disease transmission and biofilm formation. A prime challenge of swimming bacteria is to navigate in their habitat purposefully and efficiently, e.g., in the soil, which is a complex, structured environment. In this talk, we address the interrelation of bacterial navigation at the microscale and their large-scale spreading in heterogeneous environments considering both, undirected motion in a porous medium as well as biased motion in chemical gradients. We combine experiments, using the soil bacterium Pseudomonas putida as a model organism, and active particle modeling [1]. First, we examine how the disordered environment (agar) alters the run-and-turn motility patterns of these bacteria known from bulk liquid—remarkable motility characteristics, including transient subdiffusion, primarily due to intermittent mechanical trapping with power-law distributed trap times, are revealed [2]. Furthermore, we provide evidence that Pseudomonas putida performs chemotaxis in porous media, even though their mean free path is severely restricted [3]. In contrast to the well-studied case of bacterial chemotaxis in uniform bulk fluid, relying mainly on the modulation of run times in dependence on the direction of motion (run time bias), we identify a second chemotactic strategy: the change in swimming direction upon a turn event is adjusted, so that the direction of the next run phase is biased towards the source of the chemoattractant (turn angle bias). Active particle modeling, based on the experimentally inferred statistical properties of the swimming pattern, indicates that turn angle bias is the predominant chemotaxis strategy of bacteria in porous environments [3].

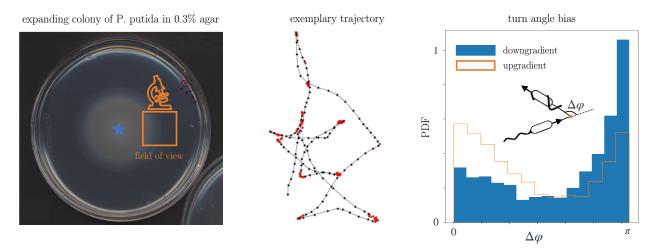


Figure 1: Left panel: expansion of a bacterial colony in agar; middle panel: exemplary trajectory of a bacterium, recorded at the edge of the expanding colony as indicated on the left; right panel: turn angle bias, *i.e.*, bacteria can tune the variation of their direction of motion in dependence of the orientation of the preceding run with respect to the chemical gradient.

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#### Fluctuation-driven Propulsion in a Self-produced Viscosity Gradient

Bokusui Nakayama<sup>1</sup>, Ryoya Hirose<sup>1</sup>, Yusuke Takagi<sup>2</sup>, Masatoshi Ichikawa<sup>1</sup>, Eiji Yamamoto<sup>2</sup>, Marie Tani<sup>1</sup>, Ibuki Kawamata<sup>1</sup>, and Akira Kakugo<sup>1</sup>

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<sup>2</sup>Department of System Design Engineering, Keio University, Yokohama, Japan

Microscale locomotion commonly relies on thermal noise. For instance, Brownian ratchets rectify stochastic motion into directed transport via asymmetric potentials. Beyond this, biological systems sometimes employ a more sophisticated strategy: actively modifying their environment to create local gradients that induce anisotropic diffusion. Certain bacteria, such as *H. pylori* and *L. monocytogenes* [1], alter their surrounding viscosity to help their Brownian bodies acquire higher motility, potentially exploiting a Brownian ratchet-like mechanism. Understanding the mechanism behind this noise-driven locomotion is of significant interest in fundamental science and also holds promise for engineering applications.

Here, we introduce a new class of self-propelled motion in an artificial system: self-viscophoresis. Unlike conventional Brownian ratchets, which rely on a phoretic drift, our system exploits self-induced local viscosity gradients to generate directed motion. While the particle consumes energy to actively modify its surrounding diffusivity landscape, its motion remains fundamentally passive, as it is driven purely by thermal fluctuations (Fig. A). This mechanism emerges an effective anisotropic diffusion, causing apparent self-propulsion. Unlike self-thermophoresis [2] and self-diffusiophoresis, self-viscophoresis originates from self-induced rheological asymmetry without requiring any explicit forces. In this work, we utilized a laser heating system (Fig. B) and a thermoresponsive polymer (Pluronic F127) solution (Fig. C) to demonstrate self-viscophoresis of Janus particles (Fig. D) as an example of self-Brownian ratchet motion.

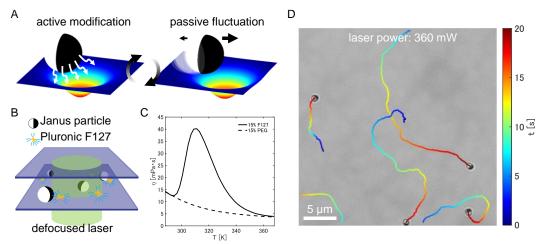


Fig. A: A conceptual illustration of self-viscophoretic motion. Fig. B: Laser heating system including Janus particles in a thermoresponsive polymer (Pluronic F127) solution. Fig. C: Temperature dependence of F127 solution's viscosity. Fig. D: The trajectories of Janus particles self-propelling under laser illumination.

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### Modeling microorganisms: Escherichia coli and Trypanosoma brucei

Holger Stark <sup>1</sup>, Pierre Martin <sup>1</sup>, Zihan Tan <sup>1</sup>

Microorganisms are around us everywhere. They occupy quite diverse natural habitats on the earth and also in the human body, where they have to navigate in complex environments such as the gut, different forms of tissue, and blood vessels. We present our efforts to model two types of microorganisms in order to understand how they move close to surfaces and in confining geometries using elastic theories and hydrodynamic simulations based on the method of multi-particle collision dynamics.

The *E. coli* bacterium uses a bundle of helical flagella driven by rotary motors, which are embedded in the cell wall, to propel itself forward. If one of the motors reverses its direction, the bundle disintegrates and the *E. coli* tumbles. It changes its swimming direction, in order to swim up a chemical gradient known as chemotaxis. In the talk we show, how the distribution of tumble angles is modified close to a surface. We observe increased tumbling in forward direction [see Fig. 1a)], where the swimming direction hardly changes [1]. This might explain the experimental finding that tumbling close to surfaces is reduced.

The African trypanosome *T. brucei* causes the life-threatening sleeping sickness. It has a spindle-shaped cell body to which an eukaryotic flagellum is firmly attached [see Fig. 1b), top]. Therefore, when a bending wave runs along the flagellum, the whole cell body is distorted and thereby propels the trypanosome forward. When injected into the skin through a bite of the tsetse fly, the trypanosome needs to move through different types of tissue before entering the blood flow and ultimately invading the brain. Thereby, it has to move in tight spaces and squeeze through narrow openings. In the talk we present how a trypanosome swims in confining geometries such as circular microchannels and how it squeezes through narrow contrictions with the help of its thin anterior end [see Fig. 1b), bottom].

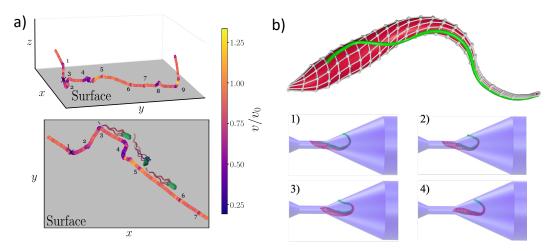


Figure 1: a) Trajectory of the model *E. coli* close to a surface; 3D representation and top view. The numbers indicate tumble events and the color encodes the swimming velocity. b) Top: Model trypanosome with the attached flagellum. Bottom: Snapshots of the model trypanosome using the anterior tip to pull the cell body out of a constriction.

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- [2] Z. Tan, J. I. U. Peters, and H. Stark, submitted to New J. Phys.; doi: 10.48550/arXiv.2412.17673

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### Symposium 3: Control and design of self-organization

Jr-shin Li, Hiroya Nakao, Riccardo Muolo

### **Curvature Analysis for Inferring Nonlinear Dynamics: Applications in Reconstructing Chemical Reaction Networks**

#### Vignesh Narayanan, Lawrence Bordoh, Istvan Kiss, and Jr-Shin Li

Inferring interpretable models of nonlinear dynamic networks (NDNs) from measurement data is a critical task across a wide range of scientific fields. A major challenge in this process is the difficulty of accurately discerning the coupling and drift dynamics of agents in an NDN from data. Efficiently solving this network inference problem requires access to data that provides sufficient information about the coupling functions, along with a well-formulated learning problem that can recover these functions without prior knowledge of the drift dynamics of the agents/nodes. This is particularly important in the context of chemical reaction networks, where quantifying interaction networks allows for the description, prediction, and control of various phenomena in chemistry and biology. However, a key challenge in this context is unambiguously attributing changes in reaction rates to specific interactions. To address this, we propose that the curvature change of kinetic trajectories, resulting from systematic perturbations to a node in the network, can be used to identify coupling. Specifically, the coupling strength can be computed as the ratio of the curvature change at a coupled node to the rate change of the perturbed node. We demonstrate this methodology through numerical simulations involving a network of complex ordinary differential equations and experiments with electrochemical networks. The results show accurate network inference, with no false positives or negatives, even in systems with significant heterogeneity in local dynamics and network structure, all without any prior knowledge of the kinetics. The theory and experiments also clarify how local perturbations influence response amplitude and timing, through network-wide upregulation.

#### Instabilities of a bimolecular reaction driven by buoyant flows

Adam Bigaj <sup>1</sup>, Luka Negrojević <sup>1</sup>, Lucie De Jong <sup>1</sup>, Laurence Rongy <sup>1</sup> 

Université libre de Bruxelles (ULB), Brussels, Belgium

Autonomous oscillations are captivating examples of self-organized behavior, observed across diverse fields such as biology, chemistry, climate science, and financial markets. Numerous complex reactions undergoing chemical oscillations have been investigated experimentally (e.g. the Belousov-Zhabotinsky and the Bray-Liebhafsky reactions) and numerically (e.g. the Brusselator and Oregonator models). In these systems, self-organization arises from the nonlinear chemical feedback, a key feature of oscillatory instability.

However, over the past few years, it has been demonstrated that local oscillations in the concentrations of chemical species can arise under isothermal batch conditions in simple bimolecular  $A + B \rightarrow C$  reactions, provided they are actively coupled with hydrodynamics. In these reaction-diffusion-convection (RDC) systems, reactant solutions initially separated in space react upon diffusive contact, producing a new species with different physical properties, thereby inducing a fluid motion. Recent numerical studies of bimolecular reactions in symmetric systems, *i.e.* where both reactant solutions share the same initial properties, highlighted that a coupling between the reaction and hydrodynamic flows (due to both density and surface tension changes) can induce oscillatory dynamics in specific cases[1-2].

Here, we present a novel approach on how to make a bimolecular reaction oscillate, both experimentally and numerically, by coupling it to chemically-induced buoyant flows. These systems, previously studied in symmetrical conditions were shown not to oscillate. However, introducing an asymmetry in the initial conditions – by considering differences in density, diffusivity, or initial concentrations between chemical species – leads to the formation of self-organized wavy patterns. The dynamics have been experimentally characterized using the oxidation reaction of fluorescin (transparent) into fluorescein (fluorescent) and further validated by numerical simulations.

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## Turing instability in reaction-diffusion systems with equal diffusion coefficients $Hirokazu\ Ninomiya^1$

In the study of pattern formation in chemical systems, Turing instability is one of the most well-known mechanisms. It describes a phenomenon where a stable equilibrium in a system of ordinary differential equations becomes unstable when diffusion is added, leading to the emergence of spatially periodic stable patterns [1]. Typically, Turing instability occurs when the reacting species have different diffusion rates. Therefore, when the diffusion coefficients are equal, the usual conditions for this instability may not be satisfied. An interesting question in pattern formation is whether Turing instability can occur when the diffusion coefficients are equal. This talk presents an example of Turing instability emerging with equal diffusion coefficients [2] and explores the conditions under which it occurs. These findings raise fundamental questions about the role of diffusion in pattern formation.

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School of Interdisciplinary Mathematical Sciences, Meiji University, Tokyo, Japan

#### **Hierarchies of Cluster States in Ensembles of Coupled Oscillators**

#### Katharina Krischer

Physics Department, Technical University of Munich, Germany

The collective dynamics of an ensemble of coupled oscillators is the key to the functioning principle of many systems in virtually all scientific fields, from neurology to energy sciences. Based on our experimental observations in electrochemical systems, I will discuss universal mechanisms that lead to the formation of hierarchies of cluster patterns in ensembles of identical or slightly heterogeneous oscillators. Particular attention is placed on organizing centers that dictate the bifurcation structure at a given level of differentiation, and on how the transition from one level to the next more complex one is realized. I will illustrate that the dynamics follow different but universal paths between synchrony and incoherence depending on the type of coupling.

### Symposium 4: Oscillation and synchronization

#### Istvan Kiss, Katharina Krischer, Hiroshi Kori

## Self-organization of optimal network formation: emerging capabilities of Physarum polycephalum

<u>Daniele Proverbio 1</u>, Damiano Reginato 1, Giulia Giordano 1

From micro-swimmers to social amoebas to slime moulds, complex microbiological systems often showcase amazing capabilities to self-organise and solve complex tasks in heterogeneous environments [1], through emerging behaviours that guarantee survival. Understanding the key mechanisms that ensure self-organization, and demonstrating its efficiency and optimality, sheds light onto spatial pattern formation in biological systems, and informs the design of engineered systems with desired properties, from swarms of robots to decentralised algorithms.

This talk focuses on the slime mould *Physarum polycephalum*, which is characterised by impressive self-organising capabilities. For instance, it was shown to successfully solve puzzles and mazes by connecting food sources via short paths [2], link multiple food sources while avoiding risky environments [3], and optimise transport networks [4]. We use different modelling approaches to capture the mechanisms underlying its behaviour, and the associated emergent patterns. First, we use an agent-based approach to study the core behaviours that ensure the robust formation of networks connecting food sources, despite uncertainties and perturbations [5]. After observing the efficiency of the constructed networks, we further develop a non-linear dynamical model for the growth of *Physarum* in maze environments and demonstrate that the emergent networks are optimal [6].

Overall, our results provide insight into the evolution of primitive intelligence and investigate the tradeoff between biological fidelity and computational efficiency.

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## Rogue-like Waves in a Reaction-Diffusion System: Stochastic Output from Deterministic Dynamics

<u>Arik Yochelis<sup>1,2</sup></u>, Edgar Knobloch<sup>3</sup>

Rogue waves are large excitations that appear intermittently and unpredictably, arising across different scales, ranging from ocean waves through optics to Bose-Einstein condensates. Motivated by spatiotemporal dynamics in a model for branching, I will describe the emergence of rogue wave-like dynamics in a reaction-diffusion system that arise as a result of a subcritical Turing instability and in the absence of an oscillatory instability [1]. This state is present in the regime where all time-independent states are unstable, and consists of intermittent excitation of spatially localized spikes, followed by collapse to an unstable state and subsequent regrowth. Characterization of the spatiotemporal organization of spikes shows that in sufficiently large domains, the dynamics are consistent with a memoryless process. Since the Turing instability is a generic pattern-forming instability of reaction-diffusion models, the results reveal a generic mechanism that sheds fresh light on time-dependent patterns in physicochemical and biological applications.

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### Si Electrodissolution as a Model System for Collective Oscillatory Behavior: Theory and Experiment

Yukiteru Murakami<sup>1</sup>, Nicolas Thomé<sup>1</sup>, Katharina Krischer<sup>1</sup>

<sup>1</sup> School of Natural Science, Physics Department, Technical University of Munich, Garching, Germany

The anodic oscillation of silicon electrodissolution in a fluoride-containing solution is a prototypical model system for studying various types of collective behavior in oscillatory systems with its unique global and nonlocal coupling mechanisms.

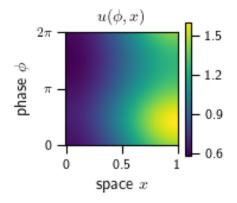
In the first part of this talk, I will present a physical model of this Si oscillator. The oscillations involve the formation and dissolution of an SiO<sub>2</sub> layer at the interface between the Si bulk and the electrolyte. An essential variable of the model is the concentration of defects in the SiO<sub>2</sub> layer, such as oxygen vacancies and partially oxidized SiO, which are created at the Si/oxide interface, slowly travel across the oxide layer, and are finally etched at the oxide/electrolyte interface. From a certain oxide layer thickness on, the traveling time between defect creation and dissolution exceeds a critical time delay, which destabilizes the steady dissolution rate in a Hopf bifurcation and thus induces limit cycle oscillations.

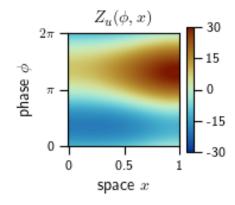
Furthermore, I will highlight the emergence of amplitude clusters from a uniform oscillatory state in the presence of a global coupling, which is introduced by an external resistor connected in series to the electrode. I will discuss how the relative ratio of the areas covered by the two regions with different amplitude changes with the global coupling strength and compare the experimental dynamics with theoretical results from the complex Ginzburg-Landau equation with global coupling.

## Understanding and Controlling Oscillatory Patterns in Reaction-Diffusion Systems with Delay by Developing Phase Reduction Method

Ayumi Ozawa <sup>1</sup>, Yoji Kawamura <sup>1</sup>

Delay can induce oscillation in dynamical systems. In particular, partial differential equations with delay often have stable oscillatory solutions and are used to model oscillatory patterns in nature. While the bifurcation theory unveils the condition under which such oscillatory patterns arise, it remains difficult to analyze how the oscillatory patterns respond to perturbations such as external forcing, interaction with other systems, and noise. To fill this gap, we aim to formulate phase reduction methods [1] for partial differential equations with delay. Specifically, in this presentation, we reduce reaction-diffusion equations with discrete delays into phase equations that describe the modulation of the rhythm by perturbation. As an example, we consider the one-dimensional Schnakenberg system with delays [2] in the oscillatory regime (Fig. 1a). The theory enables us to obtain the phase sensitivity function, which quantifies how the rhythm of the oscillatory pattern is modulated depending on where and when the perturbation is applied (Fig. 1b). We also demonstrate that a variety of mathematical tools for phase equations, including an optimization method for mutual synchronization [3], can be immediately applied once the reduction is conducted. Thus, our theory enhances the analyses and control of oscillatory patterns induced by delay.





- (a) The oscillation of the distribution of a component u is illustrated for one cycle.
- (b) The *u*-component of the phase sensitivity function,  $Z_u$ , is spatially non-uniform and varies with phase.

Figure 1: Phase reduction of one-dimensional Schnakenberg system with delay.

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### Inverse problems related to pattern formation on coupled oscillator networks $Oleh\ Omel'chenko\ ^1$

Mathematical models describing the collective behavior of large populations of coupled phase oscillators can be found in various fields of physics, chemistry, and biology. In the thermodynamic limit, when the number of oscillators N tends to infinity and the distribution of oscillator parameters converges to some probability density, it is often observed that after a sufficiently long transient, the state of the population approaches some statistical equilibrium [1,2,3]. In this talk, we describe how the properties of this equilibrium can be used to reconstruct system parameters of the underlying network. The effectiveness of the approach is demonstrated by its application to so-called chimera states in networks of phase oscillators with nonlocal coupling [4].

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### Multiple oscillation frequencies in slime mold transportation networks and its relation to chimera states.

#### Atsuko Takamatsu <sup>1</sup>

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The chimera state, a phenomenon wherein a homogeneous system of oscillators can exhibit an inhomogeneous state consisting of synchronized and asynchronous clusters of oscillators, has garnered significant research interest since its theoretical introduction by Kuramoto and Battogtokh in 2002 [1, 2]. This study presents chimera-like spatiotemporal oscillation patterns observed in the plasmodial slime mold *Physarum polycephalum*. This is a large unicellular organism that develops a transport tube network that facilitates the distribution of protoplasm throughout the cell body, thereby inducing oscillations in thickness among the partial bodies (Fig. 1a). During network formation, the oscillation pattern changes. Initially, the spatial distribution of the oscillation frequency was nearly uniform and subsequently transitioned to clusters of multiple frequencies (Fig. 1b-d). Notably, the bifurcation point aligns with the behavioral transition. This phenomenon is compared with chimera states using a simplified coupled oscillator model, wherein oscillators are posited to exhibit simultaneous positive coupling at short distances and negative coupling at long distances. The former mimics the diffusion of chemical substances within the protoplasm, whereas the latter results from the pressure differential between protoplasm at two distinct sites connected by a transport tube. The system demonstrated frequency bifurcation depending on the network size, similar to the observations in the slime mold.

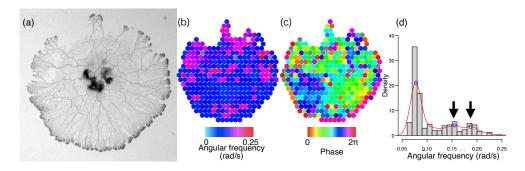


Figure 1: Tube network in slime mold (a). Spatial distribution of oscillation frequencies (b) and phase (c). Multiple frequencies (d).

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## Bistability between synchronization states at strong coupling due to higher order interactions

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Coupled oscillator networks often display transitions between qualitatively different phaselocked solutions—such as in- and anti-phase oscillations—following perturbation or parameter variation. In the limit of weak coupling, these transitions can be understood in terms of commonly studied phase approximations. As the coupling strength increases, however, predicting the location and criticality of transition, whether continuous or discontinuous, from the phase dynamics may depend on the order of the phase approximation—or a phase description of the network dynamics that neglects amplitudes may become impossible altogether. Here we analyze synchronization transitions and their criticality systematically for varying coupling strength and interaction time-delay in theory and experiments with coupled electrochemical oscillators. Two sets of experiments are presented. In the first, with oscillator close to Hopf bifurcation, phase models predicted an abrupt transition from into anti-phase oscillations as the coupling delay varied. Instead, bistability between in- and anti-phase oscillations were observed. In the second, with moderately nonlinear oscillators (far away from Hopf bifuraction), phase models predicted a continuous transition between out-of-phase and anti-phase oscillations Instead, bistability between the two states were observed. For both experiments, we analyze the bifurcations with higher-order phase models and discuss conditions under which synchronization transitions with different criticalities are possible. Our results showcase that reduced order phase models may miss important features that one would expect in the dynamics of the full system.

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### Symposium 5: Pattern formation and biological self-organization

### Martin Falcke, Hiroyuki Kitahata

# From cell motility to collective behavior around topological defects: a bottom-up approach to decrypting tissue dynamics

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Monolayers of confluent elongated cells are frequently considered active nematics, featuring topological defects. In extensile systems, where cells extend further along their long axis, they can accumulate at +1/2 defects and escape from -1/2 defects. Nevertheless, collective dynamics surrounding integer defects remain insufficiently understood. We induce diverse +1 topological defects (asters, spirals, and targets) within neural progenitor cell monolayers using microfabricated patterns. Remarkably, cells migrate toward the cores of all +1 defects, challenging existing theories and conventional extensile/contractile dichotomy, which predicts escape from highly bent spirals and targets. By combining experiments and a continuum theory derived from a cell-level model, we identify previously overlooked nonlinear active forces driving this unexpected accumulation toward defect cores, providing a unified framework to explain cell behavior across defect types. Our findings establish +1 defects as probes to uncover key nonlinear features of active nematics, offering a methodology to characterize and classify cell monolayers. This approach also reproduces the dynamic responses of the system to external stimuli.

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### Behavioral Patterns of Protists in Relatively Complex Experimental Environments

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The natural environment in which protists live is not uniform in space and not stationary in time, as it contains various fluctuating factors. How individual protists behave in such real environments is an interesting question from the perspective of the ability of protists to respond to situations, and more generally from the perspective of the ability of cells to process information. As a first step towards this, we are investigating the behavior of protists in relatively complex experimental environments. In particular, we call the experimental environment that incorporates a limited but part of the complexity of the field environment a 'diorama environment', and emphasize its importance. In this presentation, we will introduce the fact that the slime mold *Physarum polycephalum* shows diverse behaviors at the individual level in a similar diorama environment. Specifically, we will introduce the environment where many tiny food grains are scattered here and there, and the situation where a weak poison is encountered on the way through a long and narrow lane. We will also introduce the diversity of individual-level behavior seen in the phototaxis of the microscopic algae Chlamydomonas, with a focus on the fact that planktonic protozoa generally swim in a spiral trajectory. We will conclude with a discussion of the role of diversity in behavioral patterns.

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## The universal speed-persistence relation of cells moving on 1D fibronectin lanes is biphasic

<u>Marcel Eberhard 1</u>, Gerlinde Schwake 2, Joachim Raedler 2, Martin Falcke 1

Eukaryotic cells migrate for many reasons: in processes such as wound healing and immune responses and during embryonic development. The migration of cancer cells leads to deadly metastases. Therefore, motility is an essential ability required by many different cell types. Beyond the variability among different cell types the motion characteristics of cells within one cell line are diverse: cells move at different speeds, some are more persistent, others hardly move. We observe cells that maintain a constant length, whereas others periodically change their length even as they moving. Additionally, cells can spontaneously transition between these states: they may start or stop moving, change directions, or begin or cease oscillating - all occurring without any external stimuli or obvious signaling events. These observations manifest the so-called multistability of morphodynamic states of cell motion. Despite this variability two general relations of cell motion were suggested: the biphasic adhesion-velocity relation and the universal correlation between speed and persistence (UCSP). The adhesion-velocity relation states that cells move the fastest, if the adhesion strength is intermediate, which has been shown for many different cell types. The UCSP correlates the speed of cells with their ability to move in one direction and it was previously reported to be monotonous: the faster the cell moves, the less likely it changes its direction [1]. However, our latest findings on 1D motion of MDA-MB-231, MCF-10A and RPE1 cells suggest that the universal speed-persistence relation is also biphasic, showing a pronounced decrease of persistence at large velocities. This biphasic relation is also predicted by our mechanical model of 1D cell motion, which already offers explanations for the biphasic adhesion-velocity relation, multistability and state transitions [2].

At the core of this model are the force balance at the leading edge and the noisy clutch of retrograde flow friction. Cell motion starts with the polymerization of actin, which pushes the membrane forward against a drag force, drives the retrograde flow of the actin network against friction and stretches the cell. Direction reversals are caused by the protrusion competition between the front and back protrusion: noise causes the back to pull, indicated by the formation of a back protrusion with increased friction, which slows down retrograde flow. If the friction at the back exceeds the friction at the front, the cells changes its direction. We show that cells at intermediate speed exhibit the most asymmetric protrusions rendering sufficiently strong back pulling unlikely, such that the statistics of noise-induced direction reversals causes a biphasic speed-persistence relation.

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#### Curved Boundaries Drive Large-Scale Rotational Motion in Algal Bioconvection

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Suspensions of swimming microorganisms can spontaneously generate large-scale currents, resulting in intricate and dynamic flow patterns. These flows are characterized by dense, cell-rich downwelling plumes interspersed with broad, low-concentration upwelling regions. Such large-scale hydrodynamic instabilities, termed bioconvection, arise from the microscopic behaviors of cells. This phenomenon was first observed in bottom-heavy microalgae like *Chlamydomonas reinhardtii* (CR), where the center of mass is located behind the hydrodynamic center of resistance. This configuration induces a gravitational torque that biases cell movement upwards, a behavior known as gravitaxis, causing bottom-heavy cells to accumulate near the surface. Due to the CR cells being approximately 5% denser than the surrounding fluid, this accumulation leads to gravitationally unstable stratification, resulting in the development of plumes and convective rolls, similar to Rayleigh–Bénard convection.

In this work, we investigate the effect of curved boundaries on bioconvection patterns in CR cells. Our experiments reveal large-scale rotational motion of bioconvection patterns in the presence of circular and spiral boundaries. To understand the underlying mechanisms, we performed numerical simulations based on the incompressible Navier–Stokes equations, incorporating a negative buoyancy term and an additional bulk stress to account for swimming CR cells, which generate force-dipoles. These simulations provided valuable insights that complemented our experimental observations.

#### Smectic-like bundle formation of planktonic bacteria upon nutrient starvation

Kazumasa A. Takeuchi<sup>123</sup>, Takuro Shimaya<sup>1</sup>, Fumiaki Yokoyama<sup>1</sup>

The majority of bacteria on the Earth live in the form of some collectives, especially as biofilms. While biofilms are usually regarded as aggregates of bacteria adhering to some surface, non-surface-attached aggregates of bacteria are attracting attention more recently and therefore less characterized.

Here, by using a membrane-type microfluidic device that we developed previously [1], we observed how planktonic bacteria *E. coli* respond to an environmental change, specifically nutrient starvation, and found that starving cells form bundle-like aggregates, with an ordering akin to that of smectic liquid crystals (see Figure) [2]. The degree of smectic-like ordering was evaluated by a deep learning approach. Conducting various experiments to identify the mechanism underlying this smectic-like bundle formation, we argue that both the depletion attraction by extracellular polymeric substances and the growth arrest, both due to nutrient starvation, are crucial for the bundle formation. Our results suggest that the physics of the smectic ordering may also be relevant to characterize some aspects of bacterial populations, especially when they are faced with harsh environments.

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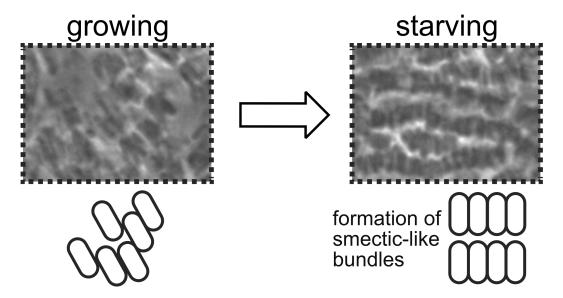


Figure: Planktonic bacteria form bundles upon starvation, with an ordering analogous to that of smectic liquid crystals [2].

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Theory of Turing patterns on discrete topologies: from networks to hypergraphs

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Nature is a blossoming of regular structures, signature of self-organization of the underlying microscopic interacting agents. Turing theory of pattern formation is one of the most studied mechanisms to address such phenomena and has been applied to a widespread gallery of applications in several domains [1]. Turing himself, in his study about morphogenesis, used a spatial discretization of the hosting support to eventually deal with a set of ODEs. Such idea, mostly overlooked in the literature, contained the seeds of the subsequent works aimed at exploring the impact of assuming discrete space. Premises of Turing patterns on regular networks date back to the 70s, however it is only with the birth of network science in the early 2000s, that the richness of dealing with a discrete support has been fully acknowledged [2]. The network based approach allows to tackle several settings which do not display a trivial continuous embedding, such as multiplex and multilayer structures [3], temporal networks [4], non-normal networks [5], and, recently, higher-order structures [6]. This line of research has been mostly confined within the community of researchers interested in network science, despite its inherent potential to transcend the conventional boundaries of the PDE based approach to Turing patterns. Moreover, network topology allows for novel dynamics to be eventually generated via a universal formalism that can be readily extended to account for higher-order order structures.

The aim of our work [7] is multiple: first, we review the main results as reported in the literature, from the Turing theory on pairwise networks to the more recent advances related to frameworks were higher-order interactions are at play; moreover, we want to introduce scholars with a physical chemistry background to the widespread realm of network applications and guide them through the advantages that it offers; lastly, we present the novel framework of higher-order interactions by extending Turing theory on hypergraphs, which are a generalization of networks. The latter is particularly relevant, as the research in this direction is only at the beginning and we believe that many exciting applications lie ahead.

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### Symposium 6: Chemical/biological information processing

### Tetsuya Kobayashi, Dimitri Loutchko

#### Controlling Biological Reaction Networks

Tetsuya J. Kobayashi <sup>1,2,3</sup>, Shuhei A. Horiguchi <sup>1,4</sup>

Biological systems across multiple scales—including chemical reaction dynamics, collective cellular behaviors, and ecological networks—can be framed as complex networks composed of interacting heterogeneous components. Chemical reaction network theory offers a unifying theoretical framework for analyzing such systems, capturing essential mathematical and physical properties. These include topological constraints derived from graph and hypergraph structures imposed by interactions, gradient flow structures originating from thermodynamic principles, and nonequilibrium dynamics governed by reaction kinetics. In this presentation, we explore how these fundamental properties of reaction networks can be applied to stochastic control problems in biological networks. Specifically, we show that by exploiting the inherent thermodynamic and information-theoretic structures of these systems, it is possible to develop a general theoretical framework for the control of nonlinear stochastic dynamics on networks. As illustrative applications, we present examples, including the regulation of molecular motors, quantitative genetic dynamics, and infectious disease control.

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## Generalized gradient systems for thermodynamically consistent modeling including temperature coupling

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In the field of ordinary and partial differential equations, gradient flows stand as a pivotal subclass characterized by their profound implications in evolution dynamics. The structured framework of gradient flows not only facilitates a deeper understanding of solution existence and stability but also unveils transformative insights into limit behaviors under parameter variations. Moreover, these flows illuminate fundamental principles governing entropy production and energy dissipation, unveiling rich geometric structures shaped by dissipation distances.

In this talk, we give an overview over the modeling of reaction-diffusion systems with generalized gradient systems  $(X, \mathcal{S}, \Psi^*)$ , where X is the state space,  $\mathcal{S}(q)$  is the entropy for the state  $q \in X$ , and  $\Psi^*(q, \xi)$  is the state-dependent dual dissipation potential with  $\xi$  denoting the thermodynamically conjugated driving force. An evolution equation  $\dot{q} = \mathcal{V}(q)$  is said to have a gradient structure if a gradient system  $(X, \mathcal{S}, \Psi)$  exists such that  $\mathcal{V}(q) = \partial_{\xi} \mathcal{R}^*(q, D\mathcal{S}(q))$ . A particular focus is on the coupling to temperature effects, where  $q = (u, \tau)$  with an arbitrary thermodynamical variable  $\tau$ , which can be for instance the temperature, the entropy density, or the internal energy. We will discuss how using a general  $\tau$  highlights the structure of the driving forces.

We discuss the notion of EDP convergence for families of gradient systems  $(X, \mathcal{S}_{\varepsilon}, \Psi_{\varepsilon}^*)$ . This convergence is based on De Giorgi's energy-dissipation principle (EDP) and allows us to study coarse-graining limits for families of gradient systems. While the driving functionals simply converge in the sense of De Giorgi's Gamma convergence, the derivation of the effective dissipation potential is more involved.

# Kinetic proofreading and higher-order replication inherited in templated ligation $Shoichi\ Toyabe^1$

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Templated ligation is a process that copies the sequence information of a template by concatenating two substrate strands. We experimentally and theoretically demonstrate that this simple information replication mode inherits a kinetic proofreading mechanism and achieves significant error suppression through cascade-manner replication [1]. In particular, the error rate at each site decreases with the length by multiplicative error suppression mechanism, which has implications for preserving genetic information in prebiotic erroneous chemistry while circumventing the error catastrophe. Notably, this process does not require complex molecular machinery for proofreading. We expect that this mechanism may also find applications in biotechnology to enhance replication fidelity. Furthermore, we demonstrate that the replication by templated ligation exhibits a higher-order nonlinear replication by autonomously forming a hypercycle-like reaction network [2]. Nonlinear replication implements the frequency-dependent selection of sequence information and can stabilize the replications of sequences without a faster replication rate, allowing the stochastic stabilization of randomly picked sequences. In particular, the coexistence of different sequences is also possible when the sequences are distributed in spatial structure. We discuss the implications of the templated ligation in the context of the origin of life and also the applications in biotechnologies to enhance replication fidelity.

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# Designing Nonequilibrium Assemblies with Reinforcement Learning and Optimal Transport

 $\underline{Grant\ M.\ Rotskoff}^{I,2},\ Shriram\ Chennakesavalu^I,\ Jérémie\ Klinger^I,\ Sreekanth\ Manikandan^I$ 

I will describe a theoretical framework for controlling the response and dynamics of nonequilibrium systems using time-dependent external couplings. These external "control protocols" satisfy a number of distinct variational principles, which become natural machine learning objective functions. The variational principles not only constrain, for example, the finite-time energetic efficiency of a given transformation, but also provide a natural objective for optimization. Finally, I will show how to solve these problems computationally for some model systems of interest, including models of experimental active matter and self-assembling actin networks.

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### Symposium 7: Fluctuations and nano-scale dynamics

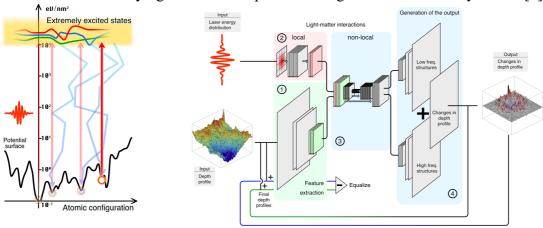
### Kazumasa Takeuchi, Holger Flechsig

### Dynamics of surface morphology driven by ultrashort laser pulses Shuntaro Tani <sup>1</sup>

<sup>1</sup> Center for Advanced Photonics, RIKEN, Japan

This talk will explore the dynamics of surface morphology induced by ultrashort laser pulses. When a femtosecond laser pulse irradiates a material surface, its intense electric field can rapidly ionize bonding electrons, triggering ultrafast structural transformations. These initial changes alter the surface morphology, which in turn modifies subsequent light-matter interactions through mechanisms such as local field enhancement, interference, and scattering. This morphology-dependent feedback leads to the emergence of complex surface structures under repeated irradiation. A prominent example of such feedback-driven pattern formation is the laser-induced periodic surface structure (LIPSS), which has been extensively studied for over six decades. However, the dynamics governing surface structure formation under multiple-pulse irradiation remain poorly understood. To address this, we experimentally investigated the transient evolution of surface morphology in a pulse-by-pulse manner and modeled these dynamics using both simplified differential equations and neural network-augmented differential equation frameworks [1].

A schematic energy diagram of the laser ablation process is shown in Fig. 1. While typical surface energies are on the order of 10 eV/nm², laser excitation can drive the system to highly excited states exceeding 10<sup>4</sup> eV/nm². This excess energy is subsequently released through laser-induced material ejection (ablation) and thermal dissipation [2], resulting in the formation of a new surface. To capture these morphological changes with nanometer precision, we employed in-situ three-dimensional microscopy in combination with laser irradiation. Our fully automated data acquisition system [3] enables the collection of tens of thousands of surface morphology datasets, providing a robust foundation for constructing a neural network-based differential equation model of surface evolution. In this framework, the neural network encodes surface morphologies into feature vectors, simulates their interaction with incoming laser pulses, and decodes the resulting vectors into predicted morphological changes. This approach enables the extraction of the underlying differential equations that govern the surface dynamics [4].



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# Partial Breakdown of the Kolmogorov–Johnson–Mehl–Avrami Theory in a Two-Dimensional Poly-Nuclear Process on the Kardar–Parisi–Zhang Kinetic Rough (001) Surface During Steady Crystal Growth

Noriko Akutsu <sup>1</sup>, Vesselin D. Tonchev <sup>2</sup>, Yoshihiro Kangawa <sup>1</sup>

The surface growth rate V during steady crystal growth is calculated using the Monte Carlo method for the (001) surface of a simple cubic lattice as a function of driving force for crystal growth  $\Delta\mu$  and temperatures T. The standard deviation of surface height W(L), where L is the linear size of the system, is also calculated to investigate the thermodynamic surface roughness. At low temperatures such as  $T < T_R^{(001)}/2$ , where  $T_R^{(001)} = 1.578\epsilon$  is the thermal roughening transition temperature of the (001) surface, the Kardar–Parisi–Zhang (KPZ) kinetic roughening transition has found by monitoring the roughness exponent  $\alpha$  (Fig. 1) [1, 2]. Here, on the KPZ kinetic rough surface, the (001) surface is atomically smooth, the surface steps are well defined, and the (001) surface grows in poly-nuclear process, though the surface is thermodynamically rough  $(W(L) \to \infty)$  as  $L \to \infty$ ).

The KPZ kinetic roughening transition point  $\Delta \mu_{\text{KPZ}}^{(001)}$  (point A in Fig. 1) has been found to agree with the crossover point between mononuclear and poly-nuclear processes [2]. From the Kolmogorov–Johnson– Mehl-Avrami (KJMA) theory, the crossover point  $\Delta \mu_{\rm DSP}$ , which is the dynamic spinodal point [3], decreases to zero in the order of  $1/\ln L$  in the limit of  $L \to \infty$ . However, in the case of the KPZ kinetic roughening, the crossover point converges to  $\Delta \mu_{\mathrm{poly}}^{*(001)}(T)$  [2] and agree with  $\Delta \mu_{\mathrm{KPZ}}^{(001)}$ within the error.

The authors wish to acknowledge Prof. Y. Suzuki and Assoc. Prof. H. Miura for their discussions. The authors also wish to acknowledge the EIG Concert-Japan. This work was partially supported by a KAKENHI Grant-in-Aid

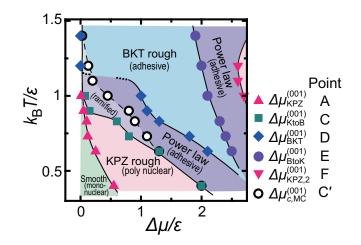


Figure 1:  $T-\Delta\mu$  Kinetic roughening diagram on the (001) surface. This figure is taken from N. Akutsu & Y. Kangawa: "Competition between Kardar–Parisi–Zhang and Berezinskii–Kosterlitz–Thouless kinetic roughening on (001) singular surface during steady crystal growth" [2] under the licence of the CC By 4.0

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<sup>&</sup>lt;sup>2</sup>Faculty of Physics, Sofia University, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

#### Exact Results in Stochastic Processes with Division, Death, and Diffusion: Spatial Correlations, Marginal Entropy Production, and Macroscopic Currents

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<sup>1</sup>The School of Mathematics and Statistics, The Open University, Milton Keynes, United Kingdom

We consider a generic class of stochastic particle-based models whose state at an instant in time is described by a set of continuous degrees of freedom (e.g. positions), and the length of this set changes stochastically in time due to birth-death processes. Using a master equation formalism, we write down the dynamics of the corresponding (infinite) set of probability distributions: this takes the form of coupled Fokker-Planck equations with model-dependent source and sink terms. We derive the general expression of entropy production rate for this class of models in terms of path irreversibility. To demonstrate the practical use of this framework, we analyze a biologically motivated model incorporating division, death, and diffusion, where spatial correlations arise through the division process. By systematically integrating out excess degrees of freedom, we obtain the marginal probability distribution, enabling exact calculations of key statistical properties such as average density and correlation functions. We validate our analytical results through numerical Brownian dynamics simulations, finding excellent agreement between theory and simulation. Our method thus provides a powerful tool for tackling previously unsolved problems in stochastic birth-death dynamics.

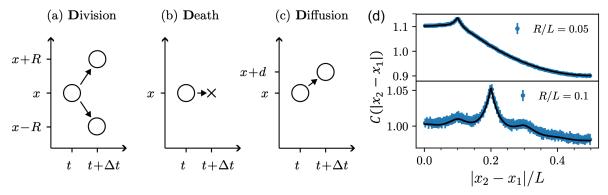


Figure: Schematic of (a) division, (b) death, and (c) diffusion processes in our model. (d) Two-body correlation function in the steady state. Markers are numerical results and solid lines are analytic results.

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Contact: elsen.tjhung@open.ac.uk

### Single-molecule Imaging of 12meric CaMKII Holoenzyme by High-speed Atomic Force Microscopy

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Structural biology reveals the three-dimensional structures of proteins at the atomic level, providing insights into their molecular mechanisms. Additionally, direct imaging of protein flexibility can enhance our understanding of protein function. High-speed atomic force microscopy (HS-AFM) is an effective technique for directly visualizing the flexible regions of single molecules under near-physiological conditions, with a temporal resolution of approximately 0.1 seconds at a nanometer resolution [1-3].

Long-term potentiation (LTP) and long-term depression (LTD) are fundamental cellular mechanisms underlying learning and memory. Functional synaptic plasticity is linked to changes in synaptic signaling strength, whereas spine structural plasticity involves modifications in the volume of the postsynaptic spine. At the molecular level, Ca<sup>2+</sup>/calmodulin-dependent protein kinase II (CaMKII) is crucial for both functional and structural spine plasticity. This 12meric serine/threonine kinase has been highly conserved across metazoans for over a million years. CaMKII is a highly abundant protein within the post-synaptic density (PSD), comparable in concentration to cytoskeletal proteins. However, the biological significance of the high concentration of CaMKII in spines and its role in the mechanisms of spine structural plasticity remains unclear. Here, we employed high-speed atomic force microscopy (HS-AFM) to visualize the molecular dynamics of CaMKIIa at the single-molecular level. In this study, we used HS-AFM to visualize the activity-dependent structural dynamics of CaMKII in rat, hydra, and C. elegans. Our results revealed that the dynamic behavior is dependent on CaM binding and subsequent pT286 phosphorylation. Notably, only rat CaMKIIa with pT286/pT305/pT306 exhibited kinase domain oligomerization. Additionally, we found that the sensitivity of CaMKII to PP2A varies among the three species, with rat, C. elegans, and hydra showing decreasing dephosphorylated respectively. The evolutionarily acquired features of mammalian CaMKIIa, in terms of structural arrangement and phosphatase tolerance, may differentiate neuronal functions between mammals and other species [4]. Furthermore, HS-AFM revealed that CaMKIIa molecules interact with each other to form clusters. To quantify the strength of intermolecular interactions within these clusters, we calculated the pair distribution function (PDF). Our results demonstrated that CaMKIIa in the basal state and in the LTP-related phosphorylation state (pT286) forms clusters through weak intermolecular interactions. Moreover, analyses of the clustering area indicated that clusters in the LTP-associated phosphorylation state are larger than those in the basal state. This suggests that CaMKIIa accumulates in the spine and contributes to the expansion of spine volume during LTP induction.

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### Fluctuation of the 3D Genome from Modeling and Experiments Soya Shinkai<sup>1</sup>

<sup>1</sup>RIKEN Center for Biosystems Dynamics Research (BDR), Kobe, Japan

Genomic DNA is hierarchically folded and compacted in the micrometer-sized cell nucleus, and its three-dimensional (3D) organization plays a crucial role in gene regulation. This architecture is inherently dynamic, continuously fluctuating over time. Understanding this "fluctuation" is essential for elucidating the relationship between genome structure and its functions.

In fixed cell populations, such structural fluctuations manifest as cell-to-cell variability. With the advent of Hi-C technology, it has become possible to indirectly infer 3D genome structures using next-generation sequencing. On the other hand, live-cell imaging enables the direct observation of real-time fluctuations in the positions and dynamics of specific genomic loci and chromatin segments.

To bridge these complementary approaches, we have developed a theoretical framework and analysis method called PHi-C [1,2,3], which integrates Hi-C and chromatin dynamics data. PHi-C employs a polymer model with linear all-to-all pairwise interactions, from which interaction parameters can be accurately inferred from Hi-C data through the PHi-C optimization algorithm. This allows for the prediction of time-resolved fluctuations at individual genomic regions, enabling integration with live-cell imaging data. As a result, we can construct a unified physical model that simultaneously reproduces both the 3D structure and dynamic behavior of chromatin in the nucleus [4].

More recently, we have shown that the motion of a single monomer within this polymer model, when compared with chromatin tracking experiments, rigorously follows a generalized Langevin equation derived from the projection method [5]. In this presentation, I will introduce our integrated modeling framework and highlight key findings on the dynamic nature of the 3D genome revealed through a combination

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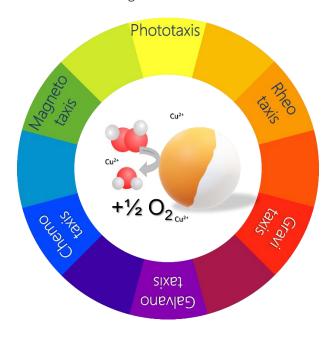
#### **Open Topics 1**

#### How smart does a material have to be to mimic biological behaviours?

#### Juliane Simmchen

#### (University of Strathclyde)

While the behaviour of biological microswimmers is undoubtedly influenced by physics, it is often controlled and manipulated by active sensing processes. Understanding the respective influences of the environment can help to engineer the desired response in artificial swimmers. In most cases, the achievement of biomimetic behaviour requires an understanding of the swimming mechanisms of both biological and artificial microswimmers and the parameters that induce mechanosensory responses. Using several examples of tactical behaviour, I will show empirical examples of how active materials can be tuned to mimic bacteria or other microorganisms.



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# Theoretical and Experimental Investigations of Some Simple Chemical Systems <u>John Smith</u>, Anna Smit<sup>2</sup>, Michael Major<sup>1</sup>

We have investigated the behavior of several simple linear chemical systems. Our investigations have shown [1,2] that their dynamics is characterized by the properties which are shared by many of them. Remarkably, we could always see that the observed behavior was decomposable into contributions coming from different involved processes. For each elementary process, a complete analytical description in terms of linear differential equations could be reached. In the future, investigations of an even larger set of simple chemical systems are planned.... The total length of the abstract should not exceed one A4 page.

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### Active Fluids with Long-Range Interactions

Itay Azizi <sup>1</sup>, Erdal C. Oğuz <sup>1,2</sup>

In this work, we ask the following question: what is the effect of long-range interactions on density fluctuations of active fluids? To answer that, we utilize molecular dynamics simulations and active matter theory. We investigate the qualitative behavior of dilute fluids of active Brownian particles (ABPs) that interact via a long-ranged power-law repulsive potential. While a passive fluid with long-range interactions exhibits anomalously suppressed long-wavelength density fluctuations, i.e., hyperuniformity, driving the fluid out of equilibrium leads to effective interactions that result in enhanced fluctuations, altered clustering and deviations from hyperuniformity. We show that the fluctuations amplitude in active systems depends on the exponent of the repulsive power-law potential, in conjunction with the spatial dimension of the system. Finally, we propose novel computational ideas for further investigation.

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# **Engineering DNA Chemical Reaction Network for Autonomous Assembly and Disassembly of Active matter**

<u>Ibuki Kawamata<sup>1</sup></u>, Kohei Nishiyama, Daiki Matsumoto<sup>2</sup>, Shosei Ichiseki<sup>2</sup>, Jakia J. Keya, Kohei Okuyama<sup>1</sup>, Masatoshi Ichikawa<sup>1</sup>, Arif M. R. Kabir, Yusuke Sato, Daisuke Inoue, Satoshi Murata<sup>2</sup>, Kazuki Sada, Akira Kakugo<sup>1</sup>, Shin-ichiro M. Nomura<sup>2</sup>

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Engineering autonomously driven active matter system from biomolecule components is of importance towards the realization of molecular-scale robots [1]. Here, we utilized microtubule propelled by kinesin molecular motor placed on glass surface as active matter [2], whose behavior is controlled by engineered DNA computing system [3]. The DNA computing system is designed to release two types of signals with a time delay, which, in turn, can assemble and disassemble the microtubules. After optimizing sample composition of DNA computing systems such as DNA, enzyme, and ion concentrations, we have successfully demonstrated the programmed time-dependent assembly/disassembly processes of microtubules without human interventions [4]. The result of fluorescent microscopy observation is further analyzed to quantify the assembly ratio, supporting our proposal of autonomous active matter. Our findings may help develop engineered biomolecular systems for various purposes such as biosensing, therapeutics, and smart material in the future.

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<sup>&</sup>lt;sup>2</sup>Graduate School of Engineering, Tohoku University, Miyagi, Japan

# Bayesian comparison of Langevin models from single tracking datasets of cell motility

Yusuke Kato <sup>1,2</sup>, Jan Albrecht <sup>2</sup>, Robert Großmann <sup>2</sup>, Carsten Beta <sup>2</sup>

This study addresses the cell motility, i.e., the spontaneous cell movement. Based on the statistical properties of experimental data, several SDE-based Langevin models of cell motility have been proposed [1,2]. However, the data-driven comparison and selection between these stochastic models have not been actively studied. Here we present a Bayesian approach to estimate and compare tentative first- and second-order Langevin models. By using the likelihood approximation technique from positional data [3], we develop a framework that ranks them based on the calculated marginal likelihood. We test and benchmark the approach using synthetic data and subsequently apply it to time-series data of Dicty cells (*Dictyostelium discoideum*) to find the best model for their ameboid motility. We evaluate the results of model selection by additional statistical analyses (e.g., MSD or velocity auto-correlation) of experimental datasets.

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# Numerical Analysis for Controlling Synchronization Transition of Chemo-Mechanical Oscillating Gels

Taro Sukegawa <sup>1</sup>, Shingo Maeda <sup>1,2</sup>

The phenomenon of synchronization plays a crucial role in several biological functions. The Kuramoto model describes synchronization transitions, where the synchronous and asynchronous states of systems switch based on the change of some parameters [1]. Experimentally reproducing this transition could enable bioinspired systems that output multiple synchronized oscillations as one large signal and control it with simple controls, such as a switch. The Belousov-Zhabotinsky (BZ) gel is a promising material for this reproduction. It deforms periodically due to its intrinsic chemical oscillations without external stimuli [2]. This property makes it suitable for the development of autonomous soft robots. However, the chemical heterogeneity in large gels makes the deformation amplitude of the gels small [3]. In addition, the high degrees of freedom in their behavior make BZ gel robots difficult to control. To address these issues, we focus on the synchronization of BZ gels, which could enable easy control of large deformations in gel assemblies. In this study, we propose a theoretical model in which multiple BZ gels are arranged in a plane under a plate connected to a movable ceiling by a spring, as shown in Fig. 1. Numerical simulations show that the synchronization and desynchronization of the gels can be easily controlled by adjusting the position of the ceiling. This approach provides a potential strategy for designing the functional deformation of bioinspired soft robotic systems with simple control mechanisms.

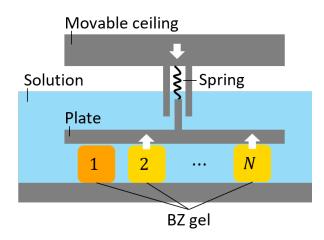


Figure 1: Overview of the system to model in this study.

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#### Harnessing any Kuramoto-like oscillator network as computational resource

Thomas Geert de Jong <sup>1</sup>, Hirofumi Notsu <sup>1</sup>, Kohei Nakajima <sup>2</sup>

Computing in silica comes with drawbacks, including high energy consumption and susceptibility to critical failures in extreme environments, such as high-radiation areas. This has sparked significant interest in discovering alternative physical systems that can overcome these limitations. Although great efforts have been made to design computer sub-components using non-traditional media, e.g., logical gates by cells [1], these approaches have not yet come close to building a functional device. A framework that overcomes this is the reservoir computing framework as it allows to directly harness the computational capabilities of a physical system without requiring a traditional computing architecture [2,3].

It has been reported that synchronization phenomenon can be utilized as a computational resource for a class of theoretical reservoir computers [4]. Even rigorous results have been put forward for a Kuramoto oscillator based reservoir [5] but unfortunately its performance is very limited in an experimental set-up. Hence, we seek an approach that is general from both the application and task perspective.

We have proposed a framework that allows for generic Kuramoto-like oscillator networks to be harnessed as a reservoir computer [6] (Fig. 1). We show by example that it can be used to perform a large variety of computational tasks for a wide range of parameters; here given by coupling and task-imprinting strength. Due to the omnipresence of physical oscillator networks our results open the door to a new class of computational device that can be designed to outperform traditional computing by physical oscillator selection.

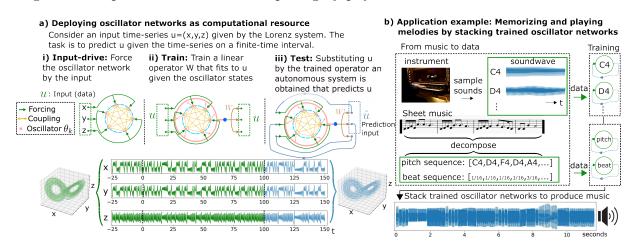


Figure 1: Framework for deploying oscillator networks with a real-world application

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### Adaptive maze solving by frozen fronts

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Unconventional computing has long sought alternative approaches to solving classical computational tasks by leveraging physical [1], chemical [2], and biological [3] systems. One of the benchmark problems in this field is maze-solving - finding the shortest path between two points in a complex environment. While numerous solutions have been proposed, each comes with limitations. For instance, wave-based solvers offer high accuracy but are relatively slow and require post-processing using classical computers [2]. On the other hand, fluidic solvers are exceptionally fast but lack adaptability due to their reliance on color indicators for path visualization [1].

In this work, we present a novel maze solver based on autocatalytic reaction-diffusion-advection (RDA) fronts, which combines the speed of fluidic solvers with the adaptability of wave-based approaches. In reaction-diffusion systems, an autocatalytic front propagates at a constant velocity, converting the reactant Y into the autocatalyst X. However, when the reactant Y is continuously injected into a cell prefilled with the autocatalyst X, a stationary RDA front forms at a fixed location where the reaction-diffusion velocity balances the opposing advective velocity [4]. This property can be exploited to solve the shortest path problem.

We show that, in a maze, the frozen RDA fronts form boundaries between viable paths and dead ends, enabling a self-organizing and adaptable approach to maze-solving. The flow from the maze entrance to the exit sustains the reactant Y in viable paths, while dead ends contain only the autocatalyst X. Changes in the flow field, due to the closure of paths or the emergence of new exits, redistribute reactants, allowing the system to find new solutions by dynamically adapting to the changing flow field. The adaptation speed is limited only by the reaction-diffusion velocity of the autocatalytic front. This approach has been validated through numerical simulations and experiments using the chlorite-tetrathionate reaction.

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### **Open Topics 2**

#### Optically and Electrically Driven Active Colloids in Liquid Crystals

<u>Ye Yuan<sup>1</sup></u>, Ghaneema N. Abuhaimed<sup>2</sup>, Qingkun Liu<sup>2</sup>, Jun-Yong Lee<sup>1</sup>, Asha Kumari<sup>1</sup>, Mykola Tasinkevych<sup>1,3</sup> and Ivan I. Smalyukh<sup>1,2</sup>

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Compared to the isotropic solvents such as water in conventional colloids, liquid crystals (LCs) as suspension media feature anisotropic elastic, fluidic and dielectric properties stemming from their collective molecular orientation. Here, we report two types of active colloids in LCs, driven by light and external electric fields, respectively [1,2]. In the first case, transparent silica microplatelets with self-assembled azobenzene monolayers undergo rotation motion when suspended in a nematic liquid crystal and exposed to unstructured 1 nW light[1]. The feedback mechanism incorporating the incident light polarization, LC director field twist, and the isomerization of azobenzene yields a continuous opto-mechanical cycle to drive the particle's unidirectional spinning; the handedness and frequency of the rotation can be robustly controlled by the polarization and intensity of the incident light. In the second case, hybrid structures formed between colloidal particles of non-trivial topology and LC solitons exhibit rotational and translational dynamics in response to alternating electric fields of different frequencies[2]. While conforming with topological theorems, the LC director distortions and topological defects within the hybrid structures may have caused the nonreciprocal evolution of the LC director fields when electric fields are applied, leading to the active motions of the hybrid structures. Our findings demonstrate various routes to exploiting the unique properties of LC molecular orientation field to construct active colloidal systems, and may contribute to the development of novel colloidal machines and micro-swimmers.

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## Numerical simulations of hexapod gait patterns by a CPG network composed of oscillatory chemical systems

 $\underline{Norihisa\ Namura}^{\ 1}\ and\ Hiroya\ Nakao^{\ 1,2}$ 

Oscillatory chemical reactions are widely observed in the real world, which can be mathematically modeled as limit-cycle oscillators. The phase reduction theory facilitates the analysis of synchronization dynamics of the oscillators by reducing the oscillator state to a single phase variable [1]. Recently, applications of oscillatory chemical systems to robotics have been studied [2]. In hexapod robots, a central pattern generator (CPG) network that mimics the mechanism for gait generation in organisms, is useful for controlling the gait patterns [3]. In this study, we construct a CPG network composed of six coupled limit-cycle oscillators and generate the phase patterns of hexapod gaits. In numerical simulations, we use the mathematical model of the Belousov–Zhabotinsky (BZ) reaction for the CPG units.

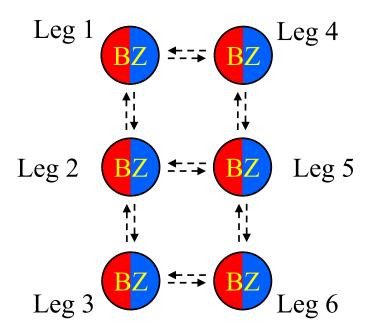


Figure 1: CPG network composed of BZ oscillators

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# Synchronization-induced Taylor's law in coupled periodic and chaotic oscillators $Yuzuru\ Mitsui\ ^{1,2},\ Hiroshi\ Kori\ ^3$

Taylor's law [1] (TL), also known as fluctuation scaling [2], is a power-law relationship between mean and variance:  $\log(\text{variance}) = \log \alpha + \beta \times \log(\text{mean})$ . When  $\beta > 1$ , this relation is called giant fluctuations in the field of active matter [3]. TL has been observed in various fields [2, 4], especially in population ecology. However, the detailed mechanisms of TL remain unclear. In particular, the underlying reasons for the widespread occurrence of TL and the frequent appearance of its exponent value close to 2 in ecosystems are to be elucidated. Here, using coupled dynamical system models, we demonstrate that TL can be induced by synchronization [5], another universal phenomenon in ecosystems. In particular, with strong coupling, time series become proportional to each other, resulting in TL with an exponent 2. Figure 1 illustrates this phenomenon in a coupled food chain model. We further confirm that these results hold for other dynamical systems, such as the Rössler model, Lorenz model, and Brusselator [5].

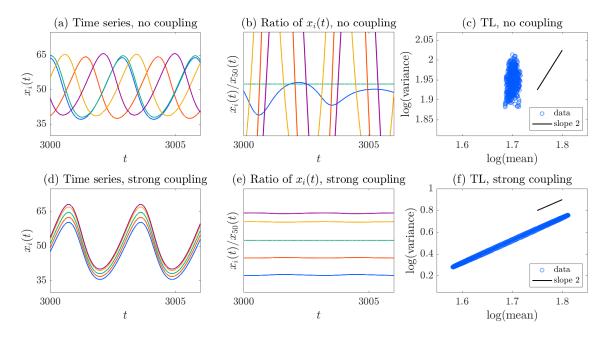


Figure 1: (a)–(c) Without coupling, the time series are not synchronized, not proportional to each other, and TL is not observed. (d)–(f) With strong coupling, the time series are well synchronized, are proportional to each other, and TL with an exponent 2 is clearly observed.

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#### Synchronization mechanism of elevators and its control

Mitsusuke Tarama <sup>1</sup>, Sakurako Tanida <sup>2</sup>

Synchronization is a ubiquitous phenomenon in nonequilibrium systems. Examples of synchronization include pendulum clocks found by Christiaan Huygens during the seventeenth century, but also biological systems such as cardiac cells, neurons, and calling frogs. One intriguing example can be found in every-day life: elevators that synchronize their motion; that is, when multiple elevators are available they tend to arrive almost simultaneously [1]. In this case, there is no direct interaction between the elevators, but they interact with each other through the (distribution of) passengers waiting at each floor.

To understand the mechanism behind the synchronization of elevators, we investigate the effective interaction between them theoretically [2]. Based on a discrete rule-based model in which new passengers at each floor appear randomly following a Poisson distribution, we show that two elevators synchronize if the influx rate of passengers exceeds a threshold value. This happens not only when the influx rate of the new passengers is uniform but also if it is biased and depends on the floors. From the obtained trajectories of the elevators, we measured phase susceptibility by assuming phase equations. Astonishingly, we found the coexistence of both attractive and repulsive interactions. By tuning the parameters of our microscopic discrete model, we were able to control the dynamical behaviour of the two elevators and realize the transition between in-phase and anti-phase synchronizations. We believe that this study provides a novel approach to design optimal transportation, which is of great importance in improving sustainable social systems.

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Network inference from synchronous oscillatory signals based on the circle map <u>Akari Matsuki <sup>1,2</sup></u>, Hiroshi Kori <sup>3</sup>, Ryota Kobayashi <sup>3,4</sup>

Synchronization is ubiquitous in nature, which is mathematically described by coupled oscillators. Synchronization strongly depends on the interaction network, and the network plays a crucial role in controlling the dynamics. To understand and control synchronization dynamics in the real world, it is essential to identify the network from the observed data. While previous studies have developed the methods for inferring the network of asynchronous systems, it remains challenging to infer the network of well-synchronized oscillators. In this study, we develop a method for non-invasively inferring the network of synchronized and desynchronized oscillators [1]. This method is based on the circle map, which describes the phase change in an oscillatory cycle. Our method discards a large part of data used for inference, which may seem counterintuitive. However, the effectiveness of the method is supported by the phase reduction theory, a well-established theory for analyzing weakly coupled oscillators. We verify the proposed method by applying it to simulated data of limit-cycle oscillators including coupled clock cells in suprachiasmatic nucleus (SCN) (Fig. 1). This study provides an important step towards understanding synchronization in real-world systems from a network perspective.

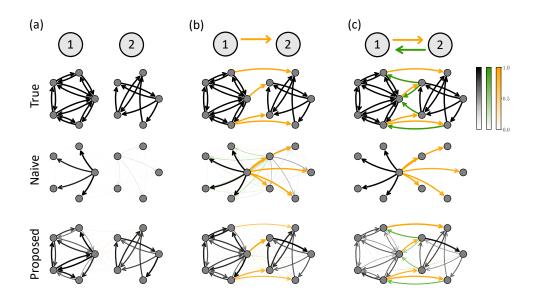


Figure 1: Network inference from oscillatory signals: Application to synthetic data of coupled suprachiasmatic nucleus (SCN) model neurons.

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# Spike generation as first passage process: Stochastic model of IP<sub>3</sub>-induced Ca<sup>2+</sup> spiking of HEK293 cells

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Biophypical theory that accounts for the stochastic character of spike sequences of IP<sub>3</sub>induced Ca<sup>2+</sup> signalling calculates the probability distributions of the features of the [Ca<sup>2+</sup>]<sub>i</sub> time course, their moments and correlations. Including slow feedbacks from  $[Ca^{2+}]_i$  to components of the pathway poses a challenge to stochastic modelling. Here, we present a stochastic model that takes these feedbacks into account, allows for a non-linear dependency of the open probability of the Inositol 1,4,5-trisphosphate receptor channel (IP<sub>3</sub>R) on the feedback variable and the inclusion of more than one feedback with different relaxation time scales. Spike generation corresponds to a first passage process in a time-dependent environment in this novel modelling approach. We use it to describe the effect of ER depletion by nonlinear rate expressions for Ca<sup>2+</sup>-induced Ca<sup>2+</sup> release (CICR) and the measured non-linear IP<sub>3</sub>-dependency of the open probability as parts of the dynamic feedbacks. Our theory can calculate spike amplitude distributions, correlation coefficients  $(C_c)$  of interspike intervals (ISIs) and amplitudes, simulate ISI distributions and calculate their moments. We apply it to experiments with HEK293 cells. We find very good agreement between theoretical ISI distributions and their moments with experimental results. Many measured  $C_c$ s show positive values in accord with the ideas formulated by our theory. Surprisingly, most ISIamplitude correlations are weak despite the decay of negative feedback during the ISI, which affects spike probability. We even find negative values of  $C_c$ s which indicate feedback that decreases the open probability of IP<sub>3</sub>R with increasing ISI. The components of the pathway causing this anticorrelation have not yet been identified. Our data suggest that they involve components that are subject to cell variability.

#### The effect of mechanical stress on pattern formation in cell spheroids

Rosalia Ferraro<sup>1</sup>, Sergio Caserta<sup>1,2</sup>, Stefano Guido<sup>1,2</sup>

The mechanical characterization of cell spheroids—one of the most commonly used 3D *in vitro* biological models—is a key area of current research focused on understanding how cells and tissues respond to mechanical forces. Although existing techniques have offered valuable scientific insights, they often require specialized equipment and technical expertise that are not typically accessible in standard cell biology laboratories.

In this context, we present some novel user-friendly rheo-optical assays enabling to apply a well-defined mechanical stress field to a cell spheroid while imaging its microstructure by optical microscopy [1,2]. Our approach allows to capture the effect of mechanical stress on the typical microstructural pattern of a cell spheroid, which is characterized by a necrotic, quiescent and proliferation zone. The results show the heterogeneous rheological properties of a cell spheroid and their dependence on biological factors, such as the cell line, the initial cell concentration, the growth time and the presence of a chemical gradient. The low-cost, user-friendly features of the proposed technique can provide novel tools in mechanobiology research making it easily affordable to any biomedical lab equipped with cell culture facilities.

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#### **POSTER SESSION 1**

#### Constructing a Statistical Mechanics Model of a Microscopic Turing Pattern

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Various spatiotemporal patterns emerge in macroscopic nonequilibrium systems, and their properties have been extensively studied using continuum field models [1]. Reaction-diffusion equations, in particular, have been widely employed to investigate patterns formed by chemical reactions. Based on these equations, Turing demonstrated that a uniform concentration field can become unstable and spontaneously give rise to inhomogeneous patterns. This Turing mechanism provides a framework for explaining a broad range of pattern formation phenomena in macroscopic systems, including morphogenesis in living organisms.

Recently, however, a Turing-like pattern was observed in a microscopic system. In Ref. [2], quantum nanowires with a thickness and width of approximately 1 nm (i.e., only a few atoms thick) were fabricated. Furthermore, it was revealed that these quantum nanowires are highly likely to have been generated by a Turing mechanism. This is a surprising observation because the continuum approximation does not hold for such small scales, and the applicability of the Turing mechanism is not obvious. To understand how Turing patterns can emerge at these scales, it is essential to consider the microscopic description of the reaction-diffusion process.

In this study, we propose a model to describe the reaction-diffusion dynamics of microscopic systems. The system consists of reaction vessels in which particles are arranged. Chemical reactions occur only between particles within the same vessel, and particles hop to adjacent vessels. Both the chemical reactions and particle diffusion are modeled as Markov jump processes. We investigate the emergence of a spatially inhomogeneous structure from fluctuations. We also compare such patterns with those obtained from the corresponding continuum models and analyze the differences between the two approaches.

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### Transition on Bifurcation Phenomena Observed in Experiments with a Rotating Elliptical Camphor Coated Disk

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A camphor boat is one of the famous self-propelled particles, which moves spontaneously on the water due to the difference in surface tension around it. The collective motions of the camphor boats resemble traffic jams and the quorum sensing in living things, and the camphor boat has been studied as an example of active matter in non-biological systems. Furthermore, the camphor boat has been an interesting topic as bifurcation phenomena, where the behavior changes drastically at a certain value of the parameter.

When an elliptical camphor disk, with the center of mass fixed at the axis of rotation, is placed on the surface of water, it rotates spontaneously. We found the appearance of the bifurcation from the stable state to the rotational state in the control of the water depth [1]. The bifurcation type, subcritical bifurcation or supercritical bifurcation, depended on the aspect ratio of the elliptical camphor disk [2]. This transition of the bifurcation type was confirmed in experiments with the control of the water depth, i.e. in the appearance of the subcritical bifurcation, the hysteresis was observed around at the bifurcation points, when the water depth increased or decreased.

We proposed the phenomenological model which includes the frictional effect between the edge of the center pore of the elliptical camphor disk and the rotational axis. The model shows the subcritical bifurcation in the existence of the friction. On the other hand, the model without the frictional effect shows the supercritical bifurcation. The results from the phenomenological model suggest that the existence of the friction determines the type of the bifurcation. We discussed dynamics in a comparison with our experimental results and simulation results obtained from our phenomenological model.

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## Calculating phase of rhythmic spatiotemporal dynamics using Poincaré section <u>Takahiro Arai 1</u>, Yoji Kawamura 1, Toshio Aoyagi 2

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The synchronization analysis of limit-cycle oscillators is prevalent in many fields, including physics, chemistry, and life sciences. Phase reduction theory [1,2] underpins an inverse problem framework to reveal causality from measurements using phase description. This enables us to identify phase coupling functions and phase sensitivity functions, which represent the linear response characteristics of the phase to perturbations. This framework requires reliable methods for calculating the phase from measurements of limit-cycle oscillators in order to model phase equations. Many studies reporting synchronization in spatiotemporal dynamics have prompted us to analyze the synchronization mechanism between the spatiotemporal dynamics. However, the inverse method to analyze the mechanism for spatiotemporal dynamics remains undeveloped. A major challenge in calculating the phase lies in the spatial complexity inherent in spatiotemporal dynamics.

Our study aims to develop a method to calculate the phase of spatiotemporal dynamics [3]. Due to the spatial structure inherent in spatiotemporal dynamics, several considerations arise for phase calculation: (i) determining the optimal locations for fixed-point observations of the dynamics; (ii) exploring the use of modes obtained from spatiotemporal dynamics through decomposition techniques such as principal component analysis (PCA) and dynamic mode decomposition (DMD).

We investigate methods that apply a Poincaré section to the time series of a measurement and utilize linear interpolation to calculate the phase. In each method, we evaluate the difference between the calculated phase and the isochron-based phase, using a linear approximation in the vicinity of the limit-cycle solution. The difference between the two phases results from the discrepancy between the isochron and the Poincaré section. Regarding (i), the difference is small when measurements are taken from regions that dominate the rhythms of the entire spatiotemporal dynamics. Regarding (ii), for both PCA and DMD, the difference depends on whether a small number of modes are sufficient to explain the phase response.

For illustration, the phase is calculated from the measurements of spatiotemporal dynamics exhibiting target waves or oscillating spots, simulated by weakly coupled FitzHugh-Nagumo reaction-diffusion models. Our study provides insight into the calculation of phase, which plays an important role in the analysis of synchronous phenomena such as atmospheric and oceanic circulation, chemical reaction systems, and heartbeats. Specifically, phase calculation requires an optimal observational approach to rhythmic spatiotemporal patterns, rather than an arbitrary observation.

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#### Circadian sinusoidal patterns as a mechanism for fluctuation suppression

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The free-running period of circadian rhythms has been reported in many studies. The period is often reported alongside the standard deviation, and variability can occur even within a single individual. For example, in mammalian cell culture rhythms, a period of  $24.38\pm1.12$  hours was reported [1], and in cyanobacteria,  $24.2\pm0.12$  hours was reported [2]. These fluctuations have been suggested to impact individual-level phenomena, such as cell transformation, aging, crop yields, and sleep. Despite this, ideas for manipulating the fluctuations of the circadian period have rarely been proposed. This is because the transcription process is incorporated into the mechanism that generates the circadian rhythm, and fluctuations in gene expression are the main cause of the fluctuations in the period. It is difficult to eliminate the effects of noise inherent in the system, and there has been no research focused on controlling these fluctuations. Does this mean that controlling circadian rhythm fluctuations is truly impossible?

To answer this question, we investigated a coupling model of the circadian clock and output system through numerical simulations [3]. As a result, we found that fluctuations in the oscillation period of the output system are significantly influenced by the waveform of the regulatory function through which the clock controls downstream gene expression. This numerical result was justified by using the theory for analytically deriving the period fluctuations of general N-dimensional oscillatory systems [4]. Furthermore, by using the results of analytical calculations to conduct sampling, we theoretically demonstrated that sine-wave-like waveforms commonly observed in circadian rhythm studies can reduce fluctuations in the output system and improve the accuracy of the rhythm.

The field of circadian rhythm research has so far focused on three parameters: amplitude, phase, and period. In contrast, this study suggests that, in addition to these fundamental indicators, the waveform itself is a new essential element of the circadian rhythm. While mutants with circadian rhythms that differ from the usual periods are known, there has been no research focusing on mutants with altered waveforms or fluctuations. Reassessing existing circadian clock mutants from the perspective of waveform could be of significant importance in controlling fluctuations in circadian rhythms.

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# Optimizing higher-order coupling for synchronization among three collectively oscillatory networks

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A networked coupling system is a complex system composed of multiple subsystems that interact through a defined coupling structure. These systems serve as essential tools in modeling a wide range of real-world phenomena, spanning domains such as biology, physics [1,2], engineering, and social sciences [3,4]. Among the various emergent behaviors observed in these systems, synchronization [5] is one of the most prevalent and crucial phenomena. It plays a vital role in sustaining the coherent functioning and stability of the overall system. Because the synchronization characteristics of a system are highly dependent on its network topology, optimizing the coupling configuration plays a critical role in reliably attaining and sustaining a targeted synchronous state, while also minimizing cost. In earlier research, Nakao et al. [6] developed an approach to optimize the coupling structures between two networks exhibiting collective oscillations, utilizing a phase-based model. Their findings revealed that tailoring the network connections in this way can enhance the speed of convergence to synchronization.

Many real-world systems, such as social networks and natural systems [7], exhibit higherorder interactions [7] involving three or more nodes. Despite their ubiquity, the study of synchronization dynamics under such complex interaction structures remains in its early stages [7]. Consequently, the direct role of higher-order coupling in synchronization control has not been thoroughly investigated, and systematic methods for optimizing these interactions are still underdeveloped.

In this study, we build upon the framework proposed by Nakao et al. [1] to investigate the optimization of higher-order coupling in a system of three collectively oscillatory networked systems. Using phase reduction techniques, we derive a two-dimensional phase difference equation that characterizes the synchronization dynamics among the three networks. Based on this formulation, we construct optimization problems that incorporate either the linear stability or rotational characteristics of the synchronized state and analytically obtain the optimal coupling tensors. Moreover, we present numerical simulations that validate and support the theoretical results.

This study contributes to the expanding field of dynamical processes on higher-order networks and offers a foundational framework for the design and control of synchronization in complex systems with higher-order interactions.

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#### Nonlinear dynamics in binary tree networks

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Complex networks and nonlinear dynamics on the complex networks have been intensively studied since the proposal of the small world and scale-free networks. The tree structure is a basic network found in various natural and social systems. The binary tree network is the simplest tree network. The bronchial network in lungs has a binary tree structure. The trachea branches into two bronchi, and the two bronchi branch into four bronchioles. We have studied some nonlinear systems on the binary tree networks. One is a reaction-diffusion-advection equation on the binary tree network as a simple model of lung. The size ratio and branching number is calculated to optimize the total reaction rate at the tips of the binary tree. The second model is coupled Lotka-Volterra equations on the binary tree. Chaotic motion induces inhomogeneity in populations at each layer, however, the long-time average of the population obeys a law of geometric series of the layer number. The third model is coupled phase oscillators on the binary tree. A chimera state appears in a certain parameter range, where a synchronized state and chaotic desynchronized state coexist on the left and right main branches of the binary tree.

#### Swarmalators that sync and divide model cleaving cell proliferation

<u>Ahmad Mohiuddin 1</u>, Oussama Ounissi 1, Thomas de Jong 1, Hirofumi Notsu 1, Ayumi Ozawa 2, Matthew Smart 3, Hayden Nunley 3

During early embryonic development in many species, a series of cell divisions transforms one cell into a cluster of tens or hundreds of cells. This often occurs by cell divisions with no growth, also known as cleaving divisions. These divisions are frequently synchronous at first but gradually desynchronize. Here, we simulate the proliferation dynamics of cleaved cells. These cells divide in a fixed domain of constant volume. We assume that the cleaved cells' shape is determined by a 2D Voronoi tesselation. Towards investigating the apparent synchrony of division events, we model the cells as oscillators with spatial degrees of freedom that are coupled to their neighbours. For the purposes of modeling the division, we assume that cells divide orthogonal to their longest axis, a phenomenon known as Hertwig's rule [1,2]. Therefore, we have a model of spatially coupled oscillators that proliferate as they complete full cycles, constituting a biologically-inspired generalization of the classical swarmalator model [3]. We explore the effect of coupling on our cleaving cell model and show that for suitable parameters the model qualitatively resembles the biology. Our future work concerns rigorous results for no finite-time blow up of divisions, dynamical systems analysis of local synchronization, connecting lineage statistics of simulations to biological experiments.

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### Selection of the thermal convection patterns in immiscible liquid bilayer with an undeformed interface

<u>Mizuki Nakamura 1</u>, Hiroaki Ito 2, Hiroyuki Kitahata 2

Rayleigh-Bénard convection is one of the most famous non-equilibrium phenomena that occur in systems with a temperature difference between the upper and lower boundaries and is driven by buoyancy caused by temperature differences. The onset of convection is determined by the Rayleigh number, a dimensionless parameter related to the buoyancy and thermal diffusion. If the Rayleigh number of the system is less than a critical value, convection does not occur. In contrast, when the Rayleigh number is above it, convection emerges.

In two-layer systems with an undeformed horizontal interface, Rayleigh-Benard convection can be coupled in two ways. The one is mechanical coupling (MC) and the other is thermal coupling (TC). The vertical flow directions in the two layers are opposite in mechanical coupling, whereas they are the same in thermal coupling[1].

We focus on the selection mechanism of thermal convection patterns in a symmetric twolayer system with an undeformed horizontal interface by varying the initial conditions in a two-dimensional hydrodynamic simulation. In this system, both the coupling patterns can be stable in a certain parameter region[2,3]. Simulations were conducted with initial conditions corresponding to each coupling pattern. Based on the simulation results, we investigated the selection mechanism of the coupling patterns. Furthermore, we discuss the specific factors determining the coupling pattern from the viewpoint of the heat transport (Figure 1).

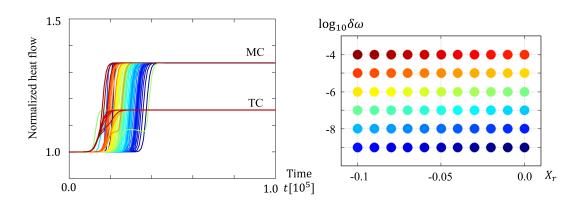


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### Long-term memory of Kuramoto oscillator based reservoir computing: Stabilizing animated GIF storage without active control

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Reservoir computing (RC) has emerged as a powerful tool for leveraging physical systems as computational resources [1]. The Omnipresent RC [2] proposes that all Kuramoto-like networks can be harnessed as devices to solve various learning tasks and forms in a sense an extension of the work in [3]. Experiments indicate promising results of Omnipresent RC for memory-tasks. However, over long time-scales instabilities can occur that destroy the systems memory. Here, we explore methods to maintain the system's stability without adding active control.

In this study, we explore the application of a vanilla type Omnipresent RC to time-dependent memorization of temporal data, specifically, we consider animated Graphics Interchange Format (GIF) images. The underlying RC equations are described by a Kuramoto model forced by a high-dimensional input corresponding to the time-series of the Animated GIF. Animated GIFs typically contain pixels that remain constant across frames, which we refer to as static pixels. Our observations indicate that during the closed-loop testing phase, oscillators linked to static pixels contribute significantly to the system's stability. In scenarios where the RC becomes unstable, augmenting the GIFs with dummy static pixels enhances the RC's performance in terms of long-term memorization. This approach suggests a novel method for addressing stability challenges in a wide range of RC applications, highlighting the potential benefits of incorporating static elements into the training data to bolster long-term memory capabilities.

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### Mathematical modeling of central pattern generator development in *Drosophila* embryos: from synchronous activity to wave-like propagation

Emiri Watanabe <sup>1</sup>, Xiangsunze Zeng <sup>2,3</sup>, Akinao Nose <sup>2</sup>, Hiroshi Kori <sup>2</sup>

Central pattern generators (CPGs) are specialized neural circuits that intrinsically produce rhythmic firing patterns and are essential for controlling repetitive motor behaviors such as walking. In the central nervous system of *Drosophila* embryos, neuronal activity begins as synchronous firing across segments around 17–19 hours after egg laying. As development advances, a temporal delay in firing emerges between adjacent segments, eventually giving rise to propagating wave patterns after 19 hours after egg laying. During the intermediate developmental phase, synchronous firing and wave-like propagation coexist [1]. While the transition from synchronous activity to wave-like patterns suggests a reconfiguration of the underlying network dynamics, the circuit-level mechanisms mediating this transformation remain poorly understood.

Here, we present a mathematical model that captures how neural networks might evolve from generating globally synchronized activity to producing segmentally coordinated wave-like propagation. By representing neurons as coupled oscillatory units, we systematically vary network topology and synaptic coupling strength to explore the emergent dynamics. We identify fundamental circuit motifs and conditions that allow synchronized and wave-like neuronal activities to coexist transiently, and that subsequently promote the emergence of propagating waves by destabilizing synchrony. These findings provide a theoretical framework for understanding how developing neural circuits may self-organize to support patterned motor outputs, shedding light on fundamental principles of circuit maturation during early embryogenesis.

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### **Light-Controlled Swarming of DNA-Modified Microtubules: Insights from Experiments and Simulations**

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Active matter systems are made up of agents that can move autonomously by converting energy from their surroundings. These systems often display fascinating collective behaviors, such as swarming and phase separation, making them promising for tasks like cargo transport and environmental sensing.

In our research, we explored an active matter system using microtubules (MTs)—tiny biological filaments that act like molecular robots. We studied ways to control the swarming behavior of MTs by attaching photo-sensitive DNA (p-DNA) to them. These modified MTs can move independently under ultraviolet (UV) and swarming and aligning under visible light, allowing us to guide their collective motion using light patterns. To gain deeper insight into this behavior, we compared our experimental results with particle-based simulations and numerical solutions of continuum equations. Our results suggest that the swarming direction of MTs can be oriented by the shape and alignment of the optical pattern. Furthermore, the effective hydrodynamic theory explains the mechanism behind the critical noise threshold at which the system transitions between ordered and disordered phases under external light field.

This research not only provides new insights into how groups of tiny biomaterials move together but also opens up possibilities for precisely controlling such swarming behavior using light.

# Flocking of the revised Cucker-Smale model with visual field

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#### Abstract

The physical description and theoretical analysis of flocking behavior have garnered significant attention over the past two decades. Researchers have focused on understanding formation mechanisms of such phenomena. In 1995, Vicsek introduced a physical model to describe collective behavior which is called Vicsek model. Later, mathematicians Felipe Cucker and Stephen Smale developed the more comprehensive C-S model. Based on the C-S framework, this research explores flocking behavior with limited perceptual abilities, particularly restricted visual field. We propose a natural and effective mathematical model to characterize these visual constraints:  $\hat{\eta} = (\frac{K}{(\sigma^2 + y)^{\beta}}) \max{\{\tilde{C}_1 + \cos\theta, 0\}}$ , where  $\tilde{C}_1$  are constants and  $\theta$  means the angle between direction of motion and position vector. When calculating the  $\cos\theta$ , we use the definition  $\cos\theta = \frac{\mathbf{v}_i(\mathbf{x}_j - \mathbf{x}_i)}{|\mathbf{v}_i| \times |\mathbf{x}_j - \mathbf{x}_i|}$ . Based on our mathematical model, we use some technical methods in the field of graph theory and dynamic system. Finally, we conducted a quantitative analysis of the sufficient conditions for the formation of flocking behavior in the C-S model with visual field. we show the one of sufficient conditions which is related to the visual field in flocking behavior:  $\Lambda(0) \leq K_{\epsilon_0}^2(0)$ , where  $\Lambda(0) = \max_{i,j} |v_i - v_j|$  at initial time point, and  $\epsilon_0(0) = \min_j \{\tilde{C}_1 + \cos\theta_{ij}\}$  at t = 0. From this sufficient condition, we are able to understand that not only does the initial energy function (or so called initial difference in individual velocities) influence the formation of flocking, but the relative positions of individuals at the initial time also play a significant role in flocking formation. This conclusion aligns with our understanding. Finally, we take some computer simulation to verify the correction of our conclusions.

Keywords: Flocking behavior, graph theory, Cucker-Smale model

Preprint submitted to Elsevier

March 29, 2025

#### Bifurcation Properties in Ultradiscrete Dynamical Systems

Shousuke Ohmori<sup>1</sup>, Yoshihiro Yamazaki<sup>2</sup>

We have analyzed the structure of bifurcation in ultradiscrete dynamical systems derived from continuous models. After reviewing the ultradiscretization method developed in the context of integrable systems [1], we examine its applications to dynamical systems exhibiting local bifurcations in low dimensions [2]–[6]. Specifically, we demonstrate that the ultradiscretization of continuous dynamical systems with local bifurcations results in bifurcations characterized by piecewise-linearity, called ultradiscrete bifurcations, which correspond to the original local bifurcations. Especially in the case of Hopf bifurcation, we found that the limit cycles emerging in continuous dynamical systems, the Sel'kov model and the negative feedback model as examples, are ultradiscretized, bringing about ultradiscrete limit cycles that consist of a finite number of states. We further revealed that such ultradiscrete limit cycles emerge due to phase lock caused by saddle-node bifurcation. Additionally, we emphasize that the Poincaré map method is highly effective in analyzing limit cycles in ultradiscrete dynamical systems.

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### Numerical and Theoretical Study on the Synchronization of the Thermal Oscillation in a Rotating Fluid Annulus

Ippei Oshima <sup>1,2</sup>, Yoji Kawamura <sup>2</sup>

Oscillations and synchronization are widely observed in chemical and fluid systems, and they have been investigated intensively [1]. One such example is the synchronization of traveling and oscillating thermal convection in a rotating fluid annulus, which has been studied through laboratory experiments [2]. The thermal convection is known as a model for atmospheric circulation and possesses both spatial and temporal phases. However, in experiments where a spatially uniform external force is applied to the outer wall, the system can be described by a limit-cycle solution characterized solely by the temporal phase.

In the present study, the synchronization of the traveling and oscillating thermal convection in a rotating fluid annulus is investigated using three-dimensional direct numerical simulations [3]. We examine an amplitude vacillation flow with a dominant azimuthal wave number of 3. The phase-sensitivity and phase-coupling functions are derived theoretically, revealing sinusoidal characteristics. Under periodic external forcing, theoretical synchronization criteria are established, accurately predicting the synchronization region.

We further propose an evaluation method based on the mean and standard deviation of the system's oscillation period. Three theoretical optimal waveforms are investigated: entrainment range, entrainment speed, and duty cycle. While optimizing the entrainment range and entrainment speed results in only limited expansion of the synchronization region, the maximum entrainment range is theoretically achieved at an optimal duty cycle of 50%, which is 12% broader than that of 100% duty cycle. Numerical simulations confirm these theoretical predictions, demonstrating that synchronization is enhanced by optimizing the duty cycle.

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### Reducing the complexity of phase-field models for cell motility to facilitate data assimilation

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Amoeboid motion is a salient form of cell motility, which is relevant in diverse biological processes from wound healing to cancer metastasis. To understand its underlying mechanism, experimental research has been complemented by theoretical modelling studies. Amoeboid motion involves dynamics of cell shape, position, and intracellular patterns. In the phasefield approach, an artificial field called 'phase' is introduced, enabling us to analyse the intracellular pattern formation, described by reaction diffusion dynamics, inside a moving and deformable domain of a cell. A number of phase-field models have been proposed to reproduce characteristics of amoeboid motion. However, the comparison between the models and experiments has remained mostly qualitative, because of the complexity of phase-field models. Accordingly, we aim to reduce their complexity to facilitate data assimilation with empirical results. A key part of our work is the derivation of the center-of-mass dynamics from phase-field models. By a straightforward calculation, we obtain a reduced expression of the form  $d\vec{r}/dt = F[c(\vec{x},t)]$ , where  $\vec{r}$  is the cell center of mass,  $c(\vec{x},t)$  is the intracellular concentration field, and F[c] is a functional of c. It represents the relation between the intracellular pattern and motion of the center of mass, while neglecting the cell shape. We discuss two possible applications of our reduced expression. Firstly, we may substitute experimental concentration distribution within a cell as  $c(\vec{x},t)$  to predict the center-of-mass displacement, whose comparison with the empirical data allows us to quantitatively verify the original phase-field model, such as those proposed in Refs. [1,2]. Secondly, we may construct a reaction-diffusion-like system for c that partially incorporates the effect of cell motion without the phase field. This can be done by introducing effective advection with the spatially homogeneous velocity  $-d\vec{r}/dt$ , neglecting the space dependence of the velocity field within a cell. By reducing the complexity of phase-field models, our work would enable parameter estimation in the context of cell motility, establishing the basis for systematic comparison between models and experiments.

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#### Large-scale chiral pattern formation in a population of migrating cells

<u>Masayuki Hayakawa</u><sup>1,2</sup>, Biplab Bhattacharjee<sup>1</sup>, Hidekazu Kuwayama<sup>3</sup>, Tatsuo Shibata<sup>1</sup>

Chirality induces various types of collective order in living and active matter systems. Such order formations have been studied mainly in closed systems, but the collective order that emerges in open systems where the number of elements changes over time as in living systems is currently unknown. We have previously reported that a mutant strain of *Dictyostelium discoideum* (KI cell) lacking all chemotactic activities forms traveling bands with polar order [1]. This collective behavior is attributable to tail-following behavior of cells at the contact site, termed contact following locomotion (CFL), which gives rise to a non-reciprocal cell-cell interaction. A theoretical model that incorporates the non-reciprocal cell-cell interactions successfully reproduce the observed behaviors [2]. In this talk, we report that the KI cell exhibits large-scale chiral pattern formation under an appropriate environmental condition. Using a simple mathematical model, we identify cell chirality and cell supply as essential factors for the observed patten formation and its dynamics.

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## Nonequilibrium thermodynamics of populations of weakly-coupled low-temperature-differential Stirling engines with synchronous and asynchronous transitions

Songhao Yin <sup>1</sup>, Hiroshi Kori <sup>1</sup>, Yuki Izumida <sup>1</sup>

This study examines the mechanisms of synchronous and asynchronous transitions in weakly coupled low-temperature-differential (LTD) Stirling engines, as well as the impact of these transitions on the power and thermal efficiency of the coupled system within the framework of nonequilibrium thermodynamics. It can be shown that synchronous (asynchronous) transitions increase (decrease) the power and thermal efficiency of weakly-coupled LTD Stirling engines based on quasilinear response relations between formally defined thermodynamic fluxes and forces. However, since the quasilinear response relations do not preserve the thermodynamic irreversibility, the analytical results deviate significantly from the true values near the synchronous transition point (red dashed lines in Fig. 1). Therefore, instead of analyzing with quasilinear response relations, we construct a conceptual model where the thermodynamic irreversibility of the original coupled system is preserved and the power and thermal efficiency can be analytically obtained. Numerical experiments show that the conceptual model gives more accurate results than those using the quasilinear response relations (yellow circles in Fig. 1). Bifurcation analysis for synchronous and asynchronous transitions was also performed for two-engine systems, which shows that the conceptual model roughly preserves the dynamical characteristics leading up to the synchronous transitions, while some detailed dynamical structures are lost.

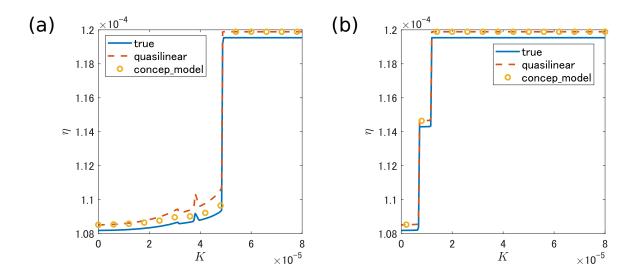


Figure 1: Dependence relation between the thermal efficiency  $\eta$  and the coupling strength K of five engines coupled in a chain with a uniform coupling strength K for (a) forward process and (b) backward process.

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#### Collective Phenomena of Active Particles Communicating through Diffusion Fields

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The collective behaviors of self-propelled agents, from bacteria to animal groups, are a central focus in active matter physics. While established models like the Vicsek and active Brownian particle models have elucidated the roles of self-propulsion, local alignment, and disorientation in shaping active matter's cooperative phenomena, the influence of chemical signaling (chemotaxis) remains relatively underexplored [1]. In colonies of chemotactic bacteria, such as Escherichia coli and Salmonella typhimurium, individual agents actively modify their environments by releasing chemical substances and subsequently adjust their behaviors in response to emergent chemical gradients. Consequently, these agents engage in indirect interactions through self-generated chemical landscapes. Unraveling how these chemically mediated interactions give rise to complex cooperative phenomena and how these phenomena manifest in living systems represents a crucial frontier.

Motivated by this, we developed a simplified model of self-propelled particles interacting through a diffusive chemical field. Our model consists of self-propelled particles and a chemical substance, represented as a continuum field  $u(\mathbf{r},t)$ . The chemical field evolves according to a diffusion equation, while the particles' motion is governed by Newton's equations with two primary forces: a constant self-propulsion force  $v_0$  and a chemotactic force that drives them towards regions of lower chemical concentration.

Analyzing this model, we observe three distinct phases dependent on self-propulsion magnitude and particle density, as depicted in Figure 1. Figure 1(a) presents a disordered phase, characterized by the absence of any long-range order. Figure 1(b) shows a hexagonally ordered phase, characterized by particles forming a crystalline-like arrangement. Finally, Fig. 1(c) presents a traveling square pattern phase, where both particles and the chemical field form a coherently moving square lattice. In our presentation, we will discuss the properties of these distinct phases and their potential relevance to living systems.

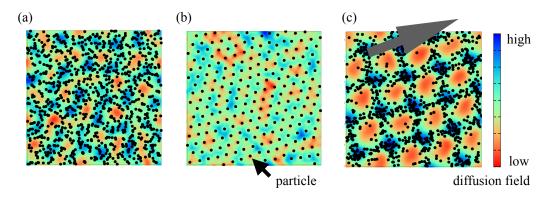


Figure 1: Typical snapshot of three phases appearing in our model. (a) disordered phase. (b) hexagonally ordered phase. (c) traveling square pattern phase. In all figures, black points represent self-propelled particles, and the background color indicates the magnitude of the diffusion field.

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#### Partitioning of embryonic domains via growing networks of coupled oscillators

<u>Matthew Smart 1</u>, Hayden Nunley 1, Ayumi Ozawa 2, Thomas de Jong 3

The robust self-organization of complex multicellular structures from a fertilized egg is a central puzzle in developmental biology. Despite the significance of this process, even the earliest steps—which involve choreographed sequences of cellular division events—remain poorly understood. Towards addressing this gap, here we propose a novel class of growing networks of oscillators, where each oscillator (cell) splits into two after completing a full cycle. Our approach conceptualizes early embryogenesis as an iterative domain tiling process, wherein successive cleavage divisions partition the embryonic volume into distinct cellular lineages. We analyze the statistical properties of these lineage tilings and identify key model parameters that govern the developmental trajectory. We further compare the resultant arrangement of the oscillators with experimental observations in model organisms and discuss experimental implications, aiming to outline promising avenues for future interdisciplinary research and the design principles of self-replicating systems.

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#### **POSTER SESSION 2**

### A Mathematical Study about the Sustaining Phenomenon of Overtone in Flageolet Harmonics on Bowed String Instruments

<u>Shodai Tanaka 1</u>, Hiroshi Kori 2, Ayumi Ozawa 3

Flageolet harmonics is a playing technique, in which a player lightly touches a nodal point on a string with their finger. Previous studies have reported that the harmonic sound sustains for a short time when the finger is removed from the string after flageolet harmonics is performed on bowed string instruments. However, little has been investigated about the mechanism of this harmonics-sustaining phenomenon and the parameter dependence of its sustaining time. We devise a mathematical model by incorporating the effects of bowing and touching into a one-dimensional wave equation. The developed model reproduces the harmonics-sustaining phenomenon, and the parameter dependence of the sustaining time is qualitatively consistent with empirical observations. We find a saddle solution near a stable solution when the finger is lightly touched, and the first Fourier mode grows exponentially after the finger is removed, depending on the distance from the saddle solution. In addition, we find that the parameter dependence on the sustaining time follows the power law. In the future, the investigation of the harmonics-sustaining phenomenon involving higher harmonics which is expective to have heteroclinic connections between the saddles corresponding to different types of overtone will take place.

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#### **Evolutionary dynamics of synthetic minimal cells**

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Living systems are self-sustaining entities that continuously proliferate by taking up nutrients from their environments and converting them into membrane molecules via complex metabolic pathways, thereby promoting membrane growth and division. Understanding how such self-reproducing systems emerged and evolved is a crucial step toward unraveling the origin of life. However, since contemporary living systems consist of highly complex enzymatic networks, it is difficult to model them directly and discuss their evolutionary strategies. To address these questions, we developed an experimental approach by constructing a simplified model system (synthetic minimal cell) that captures the essential features of living systems. Based on this system, we investigate the stability of evolving living systems. Our minimal cell synthesizes catalytic molecules on the vesicle membrane using nutrients from the environment. These catalysts incorporate membrane molecules from the external solution, enabling vesicle growth and division, i.e., sustainable proliferation [1,2]. The catalysts are polymers localized on the vesicle membranes, and their activities depend on the monomer sequence in the polymers. A key feature of this system is the strong mutual selectivity between the membranes and polymeric catalysts, the pair of which is defined as a species in synthetic minimal cells. We constructed a model evolutionary scenario in which two minimal cell species compete for resources. Minimal Cell 1 consists of membrane molecule a and catalyst  $\alpha\alpha$  (dimer of monomer  $\alpha$ ); Minimal Cell 2 consists of membrane molecule b and catalyst  $\beta\beta$ . Initially, Vesicle A and B, composed of membrane molecules a and b, respectively, are prepared, and monomers  $\alpha$ and  $\beta$ , along with the membrane molecules, are supplied. Due to molecular selectivity, Vesicle A synthesizes αα on the vesicle surface and proliferates at a membrane growth rate  $\lambda_1$ , while Vesicle B synthesizes  $\beta\beta$  and grows at a rate  $\lambda_2$ . Occasionally, catalysts containing the "wrong" monomer (e.g., αβ in Vesicle A) are produced, resulting in mutant vesicles that incorporate the other membrane molecules and exhibit altered growth rates. We analyzed the fitness of the overall system —defined as the weighted average of growth rates and population fractions—as a function of selectivity (mutation rate) [3]. Our results reveal a trade-off between proliferation and species diversity. This may highlight a universal constraint on evolutionary strategies and offer a physical perspective on the origin and evolution of life.

### Alteration of Phase-Separated Field Patterns and Dynamics by Field-Coupled Vicsek Particles

Yusuke Takagi <sup>1</sup>, Takashi Uneyama <sup>2</sup>, Eiji Yamamoto <sup>1</sup>

Phase separation is a phenomenon that occurs in multi-component mixtures, where the components separate heterogeneously. For example, mixtures of saturated and unsaturated lipids generally cause phase separation into liquid-ordered and liquid-disordered domains. Under such heterogeneous conditions, the behavior of agents is influenced by differences in the physical properties of the phases [1]. Furthermore, the phase-separation patterns and dynamics of the field are expected to be influenced by the agents. Previous studies have indicated that, in the presence of passive particle-like agents, the interaction with a particular phase causes the agents to localize within domains, leading to the formation of phase-separation patterns that support them and slow down the progress of phase separation in the late stages [2]. The modification of such phase-separation patterns and dynamics by the introduction of agents is important in the structural design and production processes of materials engineering. However, the effect of active agents on the phase-separated field remains poorly understood, and investigating new phase-separation patterns and dynamics could yield valuable insights into materials design methodology.

In this study, we conducted meso-scale simulations for the dynamic behavior of a phase-separated field that contains field-coupled particles by combining the phase-field method with Langevin dynamics simulations [1]. Moreover, we modified the Langevin dynamics simulations to incorporate self-propulsion and alignment interactions, thereby modeling Vicsek particles as active agents [3]. This approach allows us to investigate the effect of the behavior of Vicsek particles on the phase-separation patterns and dynamics of the field. We find that introducing field-coupled Vicsek particles into the binary phase-separated field leads to the formation of droplet-like phases, even when the field has a composition that typically favors the formation of continuous phases. Furthermore, we analyzed the characteristic length of phase-separation patterns to investigate the dynamics of phase separation. The introduction of Vicsek particles alters the scaling law of characteristic length with respect to time, which is originally predicted by diffusion-limited systems, such as the Lishitz-Slyozov-Wagner theory. Overall, our simulations provide pioneering insight into the effect of the presence of active particles on the phase-separated fields.

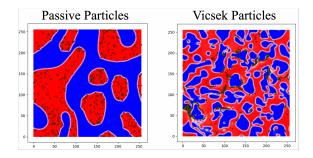


Figure 1: Snapshot of Simulations (Left: Passive particles, Right: Vicsek particles).

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### Pattern Changes of Metal Dendrites by Addition of Surfactants: Analysis on Fractal Dimension and Characteristics of Branching

Tomoya Nakamura <sup>1</sup>, Hiroaki Ito <sup>2</sup>, Hiroyuki Kitahata <sup>2</sup>

Branching patterns are widely observed in nature, from nervous systems to dendritic drainage patterns. These patterns have universal structures exhibiting self-similarity over wide scales. When a voltage is applied to an electrolyte solution, metal dendrite patterns grow from a cathode to an anode at the air-liquid interface, and the resulting dendrite size is at the order of 10 mm. Many studies have investigated macroscopic metal dendrite patterns. For example, they mainly characterized the patterns by the fractal dimension depending on various parameters[1,2]. In metal electrodeposition, including metal dendrites, the introduction of specific additives leads to interface smoothing on the scale of approximately  $10^{-2}$  mm to  $10^{-1}$  mm. For example, surfactants, quaternary ammonium salts, and polymers are known to lead to these effects. In this study, we investigated how interface smoothing at a  $10^{-1}$  mm scale affects branching patterns on a much larger scale of roughly 10 mm (about 10<sup>2</sup> to 10<sup>3</sup> times larger). We made an experiment with zinc dendrites as a model system to investigate the effects of growth-surface smoothing on large-scale dendrite patterns. Because the surfactants of the Pluronic family were reported to smooth the electrodeposition growth-interface, we added Pluronic F-127 to the zinc electrolyte solution. We examined not only the fractal dimension, which has been traditionally studied, but also quantities that characterize the shape of the pattern, such as the distribution of branch lengths and branching angles. Figure 1 shows the results of experiments. The results show that the addition of Pluronic F-127 made dendrite patterns sparse and produced the patterns with low fractal dimensions. Increasing the surfactant concentration enhanced the appearance of long branches, while the branching angles were not much affected.

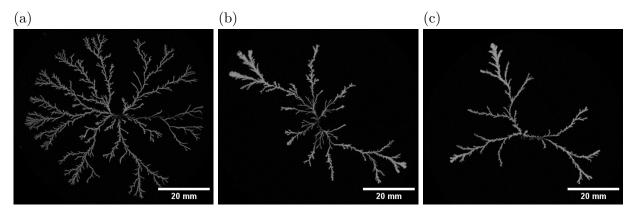


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### Reduction Methods for Spatiotemporal Pattern Formations in Non-Reciprocal Coupled Swift-Hohenberg Equations

Yuta Tateyama<sup>1</sup>, Hiroaki Ito<sup>2</sup>, Shigeyuki Komura<sup>3</sup>, Hiroyuki Kitahata<sup>2</sup>

The concept of non-reciprocity has recently attracted attention in non-equilibrium physics, including pattern formation and active matter physics, since non-reciprocity leads to novel non-equilibrium phenomena [1]. Non-reciprocity is characterized by asymmetric interactions that do not satisfy the law of action and reaction. It also induces non-reciprocal phase transitions to time-dependent phases that break space and time inversion symmetries. In recent years, the concept of non-reciprocity has been extended to gradient systems [2, 3], which are described by a free energy functional, and the bifurcation structure of non-reciprocal phase transitions has been studied [4]. The introduction of non-reciprocity into gradient systems leads to the emergence of spatiotemporal oscillatory patterns that do not appear in the reciprocal case. Several characteristic spatiotemporal patterns have been reported in the one-dimensional coupled Swift-Hohenberg equations with reciprocal and non-reciprocal linear interactions [1, 5].

This study elucidated the bifurcation structure of characteristic spatiotemporal patterns in the one-dimensional non-reciprocal Swift-Hohenberg (NRSH) model using numerical calculations and theoretical analyses based on amplitude equations [6]. The one-dimensional NRSH model is given by

$$\partial_t \phi = \left[ \varepsilon - (1 + \partial_x^2)^2 \right] \phi - \phi^3 - (\chi + \alpha) \psi,$$
  
$$\partial_t \psi = \left[ \varepsilon - (1 + \partial_x^2)^2 \right] \psi - \psi^3 - (\chi - \alpha) \phi,$$

where  $\varepsilon$  is the destabilization parameter, and  $\chi$  and  $\alpha$  are the reciprocity and non-reciprocity, respectively. Since the Swift-Hohenberg equation has a characteristic wave number of destabilization, this model's spatial Fourier modes contributing to the spatiotemporal dynamics are minimal. We derived amplitude equations for the characteristic wave number modes. We showed that the bifurcation analysis of the reduced dynamical system can understand the bifurcation structure of the characteristic spatiotemporal patterns in the NRSH model. The presentation will explain the detailed bifurcation structure, including global bifurcations, of the amplitude equation system derived from the one-dimensional non-reciprocal Swift-Hohenberg model.

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#### **Substrate Stiffness Modulates Cell Migration Speed**

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Durotaxis is a phenomenon where cells modify their migration behavior in response to substrate stiffness [1]. This behavior has been observed in many experiments including those using epithelial and cancer cells and plays a crucial role in cancer metastasis and wound healing. In this presentation, we investigate how cells crawling on a substrate respond to the stiffness of the substrate underneath using a mechanochemical model that combines intracellular biochemical reactions and cell mechanics [2]. We found that cell migration behavior changes nonmonotonically depending on the substrate stiffness (Fig.1), and we compare it with experimental observations.

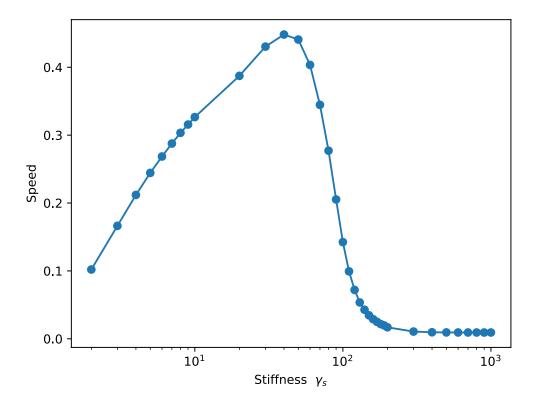


Fig.1 Cell speed at different substrate stiffness.

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#### Network Pathways influence the accuracy of circadian rhythms.

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#### **Abstract**

Circadian rhythms are essential systems that control sleep and wakefulness in various organisms, including plants, animals, and bacteria. In humans, these clocks are mainly controlled by a part of the brain called the suprachiasmatic nucleus (SCN), which adjusts our daily activities to match daylight. This adjustment is vital for keeping our bodies balanced and managing important functions like sleep, hormone release, and metabolism [1]. Similarly, in fruit flies, a network of genes, including 'period' (per) and 'timeless' (tim), creates a loop that controls the timing of protein production every 24 hours [2]. This setup helps us understand how circadian rhythms work not only in flies but also in other organisms.

However, circadian rhythms can be fluctuated by noises such as light changes, temperature shifts, and different daily routines. A recent study highlighted that fluctuations can be reduced to a certain value of the degradation rate in a simple network simulation from clock to output [3].

This research looks at how certain pathways in circadian rhythms with more complex networks can make these rhythms more precise. Using ideas from network theory, which studies how paths in networks affect their performance, we explored this using a simple model with four components representing 1 clock and 3 outputs. We ran a lot of simulations to find out which configurations keep the clock most stable. Our results show that a specific pathway that connects the clock and its output can maximally reduce noise and make circadian rhythms more precise.

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### Inferring coupling strength and frequency distribution in coupled Stuart-Landau oscillators using linear response

<u>Moonsurk Choi</u> <sup>1</sup>, Yoshiyuki Yamaguchi <sup>2</sup>

This study investigates inference of the coupling strength and the frequency distribution in a coupled Stuart-Landau oscillator system, which is a paradigmatic model of coupled limit-cycle oscillators. We analyze the system using phase-amplitude equation, which yields both phase and amplitude equations under external forces. The amplitude equation focuses on describing deviations from the limit cycle, which are utilized to infer the coupling strength from microscopic observation of time series of selected oscillators. Meanwhile, the phase equation is essential for applying a linear response theory [1,2] to infer the frequency distribution from system's macroscopic responses. In the proposed method, it is sufficient to observe only one variable among the two variables consisting of a Stuart-Landau oscillator. Through numerical simulations, we demonstrate effectiveness of this approach in inferring the key parameters. Our method offers a robust framework for inferring coupled limit-cycle oscillator systems.

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#### Activity-induced diffusion recovery in crowded colloidal suspensions

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In crowded colloidal systems, normal diffusion of colloids is observed on time scales shorter than the mean free time of collision. Sub-diffusive behavior is observed on longer time scales due to the cage effect, i.e., the mean square displacement (MSD) is not proportional to the time interval, but to  $t^{\alpha}$  (0 <  $\alpha$  < 1). On even longer time scales, diffusion becomes normal again because the colloids can escape from cages. Inside cells, diffusion is an important mass transport process, and congestion cannot be ignored. Biochemical reactions can also affect diffusion, but their effects are not obvious.

To clarify the effects of crowding and chemical reactions on the diffusion, Brownian motion in the enzyme-catalyzed reaction of urease and urea was studied [1]. The enzyme was introduced in the aqueous phase or on the surface of the particles. Experimental results showed that Both of the MSD and the index  $\alpha$  becomes greater, which indicates that diffusion was enhanced by enzyme catalysis. To discuss the detailed mechanism of diffusion enhancement, we modeled the system by two-dimensional Langevin dynamics. Enzymes are modeled as dimers, and conformational changes during enzyme-catalyzed reactions are assumed to be approximately reproduced by dimer length oscillations. We also assumed that the Brownian particles and enzymes have exclusive volumes, and they interact with each other. We numerically calculated the multi-body system of the Brownian particles and enzymes, and compared with the experimental results.

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### Seeking for Topological Edge States of Bacterial Active Matter in Asymmetric Channel Networks

Yoshihito Uchida <sup>1</sup>, Daiki Nishiguchi<sup>2,1</sup>, Kazumasa A. Takeuchi <sup>1,3,4</sup>

While active matter and biological systems are intrinsically nonequilibrium and fluctuating, the existence of topologically protected transport phenomena has been proposed theoretically using the methodology inspired by wavenumber topology in solid state physics. Recently, edge flow, i.e., unidirectional flow along the system boundary, was experimentally realized in systems composed of active particles with self-spinning or chiral motion. However, to design topological phenomena in active matter systems, it is desired to figure out a way to control the topological phenomena without changing the properties of active particles. To this end, here we aim to realize topological phenomena in dense bacterial suspension, by using microfabricated geometrical structures with nontrivial wavenumber topology. The microfabricated structures consist of wells connected by channels with an asymmetric shape, which induces unidirectional flow therein (Figure 1). In the case of asymmetric kagome networks, we find edge localization of bacterial density, which results from the characteristic collective motion of bacteria. We investigate how the bacterial flow may generate edge localization by combining the experimentally obtained velocity field and simulated particle transport. We also discuss what properties of geometrical structures are essential to designing the topological phenomena in bacterial collective motion by tuning the geometry of microfabricated structures. We expect our experimental results may pave the way for establishing a control and design principle of topological transport phenomena in such active matter systems.

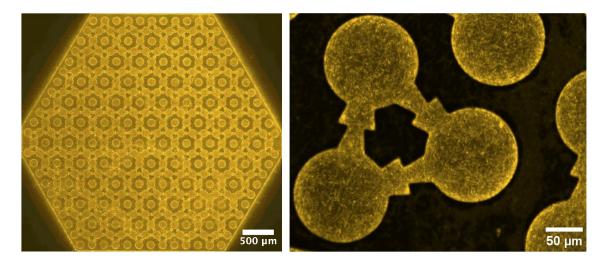


Figure 1: Confocal image of dyed bacterial suspension confined in an asymmetric kagome network (left). The kagome network is composed of wells connected by asymmetric-shaped channels showed in the right panel.

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### Asymmetric motility of micrometer-scaled soft matter under symmetric oscillatory shear

 $\underline{Tsubasa\ Yoneda\ ^1},\ Takuya\ Ohmura\ ^2,\ Yukinori\ Nishigami\ ^2,\ Hiroshi\ Orihara\ ^2,\ Toshiyuki\ Nakagaki\ ^2$ 

The behavior of soft matter systems, such as deformation and motion, is potentially relevant to cellular motility and subcellular material dynamics. We report on the non-trivial, unidirectional motion of micrometer-sized soft matter systems subjected to oscillatory shear. In experiments, we prepared a range of microscopic soft matter samples, including cell fragments, polystyrene beads dispersed in a viscous solution, and oil-in-water droplets. These were confined between two parallel glass plates and subjected to symmetric oscillatory shear at 100 Hz using a rheometer. The resulting motion of the samples was observed and recorded with a microscope attached beneath the glass plate (Figure 1a).

Analysis of the recorded videos revealed that fragments within these samples showed a consistent, unidirectional motion, occurring over spatiotemporal scales exceeding those of the applied oscillations (Figure 1b). The observed motion demonstrates the capacity of these soft matter systems to transform reciprocal mechanical input into directed translational motion. Focusing on the shapes of moving objects, we found that both beads and oil droplets formed clusters during motion, whereas a single bead or droplet does not exhibit such motion. For oil droplets, we investigated the sizes and relative positions of the droplets constituting the clusters and found that shape anisotropy in a cluster determines the direction of motion. Furthermore, by observing the flow field around oil droplets under shear and employing numerical simulations, we confirmed that these flows spontaneously induce droplet clustering. These findings raise key questions for future research: how cluster formation drives this non-trivial motion, and how it can account for the dynamics observed in beads and cell fragments.

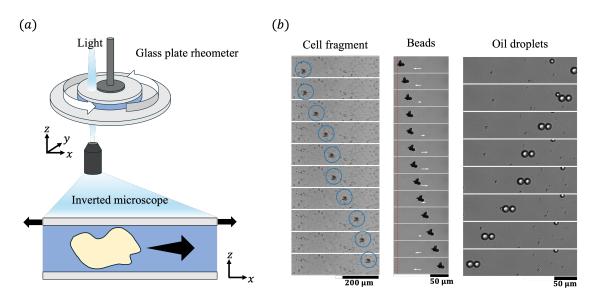


Figure 1: (a) Schematic image of experimental setup. Confined material (yellow) was subjected to oscillatory shear using a rheometer. (b) Time series of microscopic image of moving materials.

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#### Activation of nonlinear dynamical system via Lyapunov stability landscape

Motoki Nakata <sup>1,2</sup>, Masaaki Imaizumi <sup>3,4</sup>

We introduce a stochastic sampling approach to identify stability boundaries, or the edge of chaos, in general nonlinear dynamical systems with ordered and/or disordered pattern formation. The global landscape of the Lyapunov exponent in multi-dimensional parameter space is crucial for understanding transitions between stable and unstable trajectories/states in the dynamical system, whereas its analytical derivation is generally limited. To address this, we propose a computational methodology[1] that directly couples the numerical integration of nonlinear differential/difference equations with the Markov chain Monte Carlo (MCMC) algorithm, specifically leveraging an irreversible Replica Exchange MCMC (RXMC)[2]. The effectiveness of the present method is demonstrated by analyzing a chaotic neuron model[3] and the neural networks, revealing the Lyapunov stability landscape in the multi-dimensional parameter space as shown in Fig. 1. It is also shown that a posteriori modeling for the parameter subspace along the edge of chaos on the landscape can construct an inherent constrained dynamical system to activate or de-activate the chaotic trajectories or more generally the self-organization. The proposed methodology is effective for the various landscapes in a wider range of complex dynamical systems, such as magnetic fields, turbulence, and Kuramoto oscillators, even with non-differentiable or discontinuous functionals for the landscape.

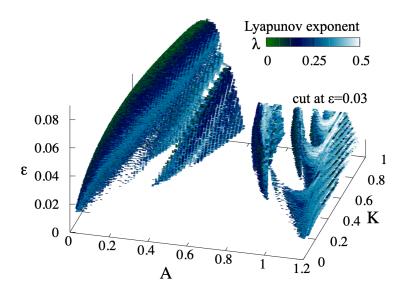


Figure 1: Lyapunov stability landscape in the 3-d parameter space for chaotic neuron model

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### Invariants of the coupled phase dynamics via Koopman operator analysis Keisuke Taga <sup>1</sup>, Hiroya Nakao <sup>2,3</sup>

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Spontaneous rhythmic phenomena observed in nature are often modeled as limit-cycle oscillators, such as the Brusselator for the Belousov–Zhabotinsky reaction and the FitzHugh–Nagumo model for neuronal dynamics. These models may be reduced to a phase model that describes the evolution of the system solely in terms of 1-dimensional phase dynamics under appropriate conditions.

In this study, we investigate invariants (constants of motion) of a class of phase models described by the following general equation [1]:

$$\frac{d\theta_j}{dt} = f(t) + g(t)\cos(\theta_j) + h(t)\sin(\theta_j), \quad j = 1, 2, \dots, N.$$
(1)

This formulation encompasses several well-known models, including the Theta model for neuronal dynamics and the Kuramoto model for synchronization phenomena.

It is known that Eq. (1) can be transformed into a Riccati equation, from which N-3 functionally independent invariants can be constructed [1,2]. An example of such an invariant is given by:

$$\frac{\sin\left(\frac{\theta_i - \theta_j}{2}\right)\sin\left(\frac{\theta_k - \theta_l}{2}\right)}{\sin\left(\frac{\theta_j - \theta_k}{2}\right)\sin\left(\frac{\theta_l - \theta_i}{2}\right)}.$$
 (2)

In this research, we consider these invariants from the viewpoint of Koopman operator theory [3]. Rather than analyzing the evolution of state variables  $x_t$  directly, Koopman analysis focuses on the time evolution of observation functions  $\phi$ , which evolve linearly under the Koopman operator  $\mathcal{K}_{\Delta t}$  given as:

$$\mathcal{K}_{\Delta t}\phi(\boldsymbol{x}_t) = \phi(\boldsymbol{x}_{t+\Delta t}).$$

For continuous-time dynamical systems governed by

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{F}(\boldsymbol{x}),$$

the infinitesimal Koopman operator is defined as

$$\mathcal{K}\phi(\boldsymbol{x}) = \frac{d\phi}{dt} = \boldsymbol{F}(\boldsymbol{x}) \cdot \nabla \phi.$$

Eigenfunctions of the Koopman operator reflect characteristic properties of the dynamics. In particular, eigenfunctions of  $\mathcal{K}$  corresponding to the eigenvalue 0 represent invariant quantities. Thus, the invariant in Eq. (2) is interpreted as an eigenfunction of  $\mathcal{K}$  associated with the phase model in Eq. (1).

We explore such invariants through the property of the Koopman operator that does not use the Riccati equation [4].

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### Selective decision-making and collective motion induced by the visual attention of fish

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Various approaches have been taken to model the fish school, but the fundamental question (i.e. how to read the positional and the temporal information of a neighbor and reflect it in own movement) is not yet fully answered. In this study, we focus on visual interaction.

We construct the equations of motion which takes into account the motion of visual attention induced by the visual stimuli from the images of the neighbors on the retina [1]. A signal is generated in each bin corresponding to a ganglion cell of the visual field, and the signals are superimposed to a synthesized signal. Next, the agent reads the position and velocity of the neighbor on the visual attention and reflects it in own movement.

In this model, the various collective patterns (e.g. the vortex pattern and the polarized school) are spontaneously emerge. Even when multiple neighbors are visible, an agent tends to track one of the neighbors rather than the average position of all agents. This result reproduces the selective decision-making in the experiment. Thus, for the first time, we have constructed a visual model that can simultaneously show the spontaneous appearance of collective patterns with several hundred agents and the experimental coincidence of selective decision-making.

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#### Spatial Distribution of Mechanical Property within 3D Bacterial Multicellular Communities

<u>Takuya Ohmura<sup>1</sup></u>, Dominic J. Skinner<sup>2</sup>, Konstantin Neuhaus<sup>3,4</sup>, Gary P.T. Choi<sup>5</sup>, Jörn Dunkel<sup>6</sup>, Knut Drescher<sup>3</sup>

Bacterial multicellular communities, biofilms, are estimated to be the most abundant biomaterial on Earth. While biofilms cause disadvantages in our lives such as clogging industrial pipes, forming dental plaque and contributing to human infections, biofilms also have been studied as living materials in bioengineering and material science. The cells within biofilms are physically combined with extracellular matrix, which gives them high resistance to chemical agents like antibiotics and makes them mechanically difficult to remove. Recent studies have revealed that cell physiological properties, including production of extracellular matrix, are spatially localized within biofilms, and this heterogeneity is observed even in early-stage biofilms. Accordingly, the mechanical properties also could exhibit localized spatial distribution, which potentially induces biofilm mechanical resistance against external force. However, there have been lacking techniques to measure the spatial distribution of the mechanical properties in living biofilms.

To investigate mechanical response of biofilms against external force, by combining microfluidic regulation, live-cell imaging, and machine learning-based image analysis [1], we observed 3D biofilm deformation under a shear flow. Tracking thousands of cells in the biofilms quantified cell displacements and orientation changes under the deformation, which showed the spatial distributions of the elastic and plastic responses inside the biofilms. By fitting the measured displacements with multi-spring models, we clarified that the elastic property gradually decreased from the inside to the outside of the biofilm, which correlated to the spatial distribution of the polysaccharides within the biofilm matrix. Our microrheological approach provides a general framework for studying mechanical properties with high spatial resolution in living materials [2].

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### Qualifying Relaxation Dynamics in Chemical Reaction Systems with Convexity Keisuke Sugie <sup>1,2</sup>, Dimitri Loutchko <sup>2</sup>, Tetsuya J. Kobayashi <sup>1,2</sup>

Chemical reaction networks (CRNs) are a class of dynamical systems widely used to model and analyze a broad range of biochemical processes. Slow relaxation in CRNs is important to better understand living cells under limited resources, and its mechanisms and characteristics have been studied. However, it remains unclear how the relaxation rates of CRNs can be quantitatively characterized by stoichiometric and thermodynamic features, as previous studies have been limited to qualitative or simulation-based approaches. In this work, we explicitly calculate the general bounds of the KL divergence in mass-action CRN dynamics for the two dissipative formulations. We exploit the convex structure of equilibrium CRNs and use convergence analysis methods in convex optimization algorithms to quantify the relaxation process. The bounds are determined by the stoichiometric singular values, the convexity indicators, and the activities of the reactions. We numerically validate the divergence bounds on specific CRNs exhibiting slow relaxation, and identify the minimal and sufficient pairs of quantities for plateau formulation.

	Gradient Flow	CRN Dynamics	
Model for	Convex Optimization	Biochemical System	
Interest	Fast Convergence	Slow Relaxation	
ODE	$\dot{\boldsymbol{x}}_t = -\alpha  \nabla  U(\boldsymbol{x}_t)$	$\dot{\mathbf{x}}_t = -\mathbb{S}[\boldsymbol{\omega}(\mathbf{x}_t) \circ \mathbb{S}^\top \nabla U(\mathbf{x}_t)]$	
$\dot{U}(\boldsymbol{x}_t)$	$-\alpha \ \nabla U(\mathbf{x}_t)\ ^2$	$-\ \mathbb{S}^{\top}\nabla U(\mathbf{x}_t)\ _{\boldsymbol{\omega}(\mathbf{x}_t)}^2$	
Control with	Learning Rate $ lpha $	Enzyme, Activity $\omega(x_t)$	

Figure 1: Comparison between gradient flows and CRN dynamics.

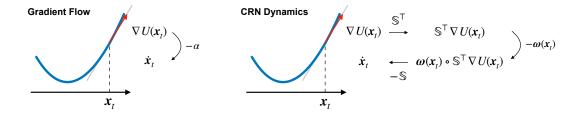


Figure 2: Convex Structures of gradient flows and CRN dynamics.

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#### Analysis of Synchronization Phenomena Using a Nonlinear State-Space Time Series Model Based on the Kuramoto Model

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The Kuramoto model is a well-known mathematical framework for describing synchronization phenomena in populations of nonlinear oscillators. In this study, we discretized the Kuramoto model and implemented it as a state-space model to analyze synchronization through the estimation of coupling strength. Specifically, we applied the ensemble Kalman filter [1] and a particle filter [2] that accounts for oscillator periodicity to estimate the coupling strength, and compared their estimation accuracy. We also quantitatively evaluated the impact of observation intervals on estimation performance. Furthermore, we conducted synchronization experiments using metronomes and estimated the coupling strength from the observed data. By comparing the results with simulations, we confirmed that the estimated coupling strength successfully captured the global dynamics of metronome synchronization.

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### Synchronization time in a ring of phase oscillators under common noise Richard Wiebe<sup>1</sup>, Hiroshi Kori<sup>2</sup>

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The behavior of periodic oscillator networks has gained attention due to their appearance in many applications across biology, chemistry, and applied mechanics. These systems present a rich family of possible responses including phase synchronization, which is a commonly-observed characteristic of systems. Many insights have been gained for the case of deterministic forcing (and system parameters), however, the inevitability of noise in real-world systems has also motivated the study of stochastic forcing scenarios. Often, the question of interest is the robustness of underlying deterministic response types to increasing noise levels. However, the special case of common noise has been demonstrated to promote synchronization, i.e. it can have a constructive rather than destructive influence<sup>1</sup>.

This work focuses on the interaction between coupling, which has also long been known to induce synchronization, and common noise. The case study is a ring of phase oscillators. Studies especially relevant to the work herein are the common noise-induced synchronization of: uncoupled limit-cycle oscillators<sup>1</sup>; globally-coupled nonidentical oscillators<sup>2</sup>; and a coupled two-oscillator system<sup>3</sup>. These studies reinforced that common noise promotes synchronization, however, the latter study indicated that the interaction between coupling and common noise is more. This work extends that, using numerical methods, to a larger ring system. The characterization method used to determine the effect on synchronization is the synchronization time vs. the coupling strength and noise level.

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#### Collective dynamics of beads on a cellular carpet

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We present a non-equilibrium multi-component system composed of motile amoeboid cells and passive beads [1,2]. The dynamics of particles is driven athermally by the motility of cells, which form an underlying active carpet. In this system, the dynamics of individual beads is characterized by spatio-temporally heterogeneous diffusion with non-Gaussian displacement distributions due to the non-uniform activity of cells [3]. In this contribution, we are particularly focusing on the collective dynamics of densely packed particle ensembles, a regime in which steric hindrance dominates the dynamics. We characterise the structural properties of the system based on experimentally recorded trajectories of beads with single-particle resolution. Spatio-temporal correlations, emergent local structural motifs, and their temporal dynamics are investigated. Thereby, we contribute to understanding the athermal, activity-mediated mechanics of passive beads driven far from thermodynamic equilibrium.

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