

Scientific Report



Theoretical and computational modeling
of complex systems

Dr. Márcio Sampaio Gomes Filho



Supervisor: Nathan Jacob Berkovits

FAPESP

Process: 2023/03658 – 9

Project period: 01/08/2023 to 31/08/2024

Reporting period: 01/08/2023 to 20/11/2023



1 Abstract

This project aims to use theoretical and computational modeling, along with machine learning methods, to gain deeper insights into the fundamental behavior of matter and uncover new physical phenomena. Depending on the system of interest, we will employ different methods ranging from classical analytical techniques to quantum mechanical simulations or complex numerical simulations. One specific goal is to develop deep neural network force fields (NNFFs) trained on small systems, which will be used to scale up to larger systems and longer time scales to investigate the properties of water in different phases, containing salts, and the properties of ice/water interface. Furthermore, we aim to address fundamental problems in characterizing the dynamics of mesoscopic systems out-of-equilibrium, including the universal growth phenomena described by the Kardar-Parisi-Zhang (KPZ) equation, and the entropic effects of confined polymer chains.

2 Undertaken activities

During the reporting period, the postdoc presented (oral presentation) the work titled "*Modeling the diffusion-erosion crossover dynamics in drug release*" at the Brazilian Workshop on Soft Matter/ICTP-SAIFR. This workshop took place in São Paulo, SP, Brazil, from October 04 to 06, 2023.

Furthermore, the postdoc participated in different projects. For instance, he had the valuable opportunity to revisit previous projects, including the investigation of entropic effects on confined polymer chains through Brownian dynamics simulations. This project, developed in collaboration with Professor Eugene M. Terentjev from the University of Cambridge (Cavendish Laboratory), had been temporarily halted during the COVID-19 pandemic.

Additionally, the postdoc initiated new collaborations with ICTP-SAIFR partners. For example, including Danilo Liarte and Pablo de Castro. Together, we embarked on a project exploring the movement of active and passive particles in an elastic network.

The following sections provide some details about the work done during the period covered by this report.

2.0.1 Using Neural Network Force Fields to obtain the structural properties of the hexagonal ice

The first project constituted an extension of our previous research [1], where we focused on determining the optimal size and quality of the training dataset for constructing a precise NNFF for liquid water. Subsequently, we analyzed the properties of hexagonal ice (ice I_h), commonly known as ordinary ice or frozen water, during this investigation. This solid phase

of water exhibits many interesting properties that are relevant to the existence of life and regulation of global climate [2].

In particular, we have investigated the structural properties of ice I_h as described by deep NN force fields for water, by comparing a set of four different exchange correlation potentials used in the training (PBE, optB88-vdW, vdW-cx, SCAN) [3]. We are currently in the process of analyzing the latest results and writing a paper.

This work has been done in collaboration with Lucas T. S. de Mirandas (IFT-UNESP), Prof. Alexandre R. Rocha (IFT-UNESP), and Prof. Luana S. Pedroza (UFABC).

2.0.2 The solvation of NaCl in water by neural-network-based molecular dynamics simulations

Electrolyte solutions are important in a variety of disciplines, from energy storage design to biological processes. However, they are still not completely understood, and many facets of studying them are computationally intensive [4]. Here, we utilize a machine learning deep potential framework to efficiently study the solvation of NaCl in water based on density functional theory. We characterize the solvation process by the potential of mean force (PMF) [5] between the solute particles, and investigate structural effects the solute (NaCl) has on the solvent (H_2O).

This collaborative research project involved the contributions of Alec Wills and Prof. Marivi Fernández-Serra from Stony Brook University, USA, as well as Prof. Luana S. Pedroza (UFABC).

2.0.3 The properties of the Ice/Water interface

We have initiated a new collaboration with Professors Alexandre Reily Rocha (IFT-UNESP, Brazil) and Maurice de Koning (IFGW/UNICAMP) with the goal of developing a neural network (NN) potential to investigate the dynamics and thermodynamics of the ice/water interface. Our primary objective is to determine the melting temperature of the ice/water phase.

At this stage, we have already developed an accurate new NN capable of describing the ice/water interface. The next step involves performing molecular dynamics simulations to investigate the dynamic properties of the ice/water interface. To characterize the thermodynamic properties, I will have the opportunity to learn how to obtain free energy curves from molecular dynamics simulations during a visit to Professor Maurice de Koning at IFGW/UNICAMP from November 20 to 25, 2023.

2.0.4 Universal geometric properties of the Kardar-Parisi-Zhang equation in $d + 1$ dimensions

The Kardar-Parisi-Zhang (KPZ) equation has been a highlight in statistical physics because it is connected to a large number of important stochastic processes in physics, chemistry and growth phenomena, ranging from classical to quantum physics. There are two central quest in this field the search for ever more precise universal growth exponents and the absence of a fluctuation-dissipation relation (FDT) for space dimensions $d > 1$. Notably, both the exact growth exponents and the FDT are only known for $1 + 1$ dimensions.

In this work, we are investigating the FDT for the KPZ equation, and its relation with fractal dimensions associated with the dynamics of growth. We already find that a new noise with a fractal dimension d_n arises naturally from the dynamics. By using geometric analytical methods that directly associate these exponents to the fractal dimensions d_n and d_f of the rough interface, we determine the growth exponents for the $2 + 1$ dimensions.

This work has been carried out in collaboration with professor Fernando A. Oliveira (IF-UnB). Professor Fernando will also visit ICTP-SAIFR/IFT-UNESP in December/2023. Our goal is to finish this collaborative project.

2.0.5 Entropic effects of confined polymer chains

Understanding the forces (or pressure) exerted by a polymer chain in confined spaces is a fundamental problem in polymer science, which has many implications in different biological processes, such as protein folding under confinement conditions, forces required to package (or eject) biopolymers (*e.g.*, DNA) into (from) a bacteriophage capsid [6]. Much of these intriguing phenomena are associated with the spatial constrains that imposes a reduction in the number of allowed configurations, resulting in the reduction of the conformational entropy, which promotes a free energy excess. Thus, the confinement free energy is only determined by the entropic effects.

In this way, a polymer chain confined in a cavity between two parallel walls (a slit) is a classical fundamental problem that reveals the essential physics. Much of developments have been take place using different approaches, for example, from theoretical scaling predictions and analytical theories for an ideal (or Gaussian) chains. On the other hand, the theory for a flexible polymer chain in a good solvent (self-avoiding chain) is much more complicated due to the pair-interactions (excluded-volume). The seminal contributions were achieved by Pierre-Gilles de Gennes (nobel prize), Sam F. Edwards (Boltzmann medal) and Paul John Flory (nobel prize) [7].

With respect to computational modeling, it is easy to simulate a chain in a confined space and determine its statistical parameters such as the radius of gyration, but it is not straightforward to find the free-energy related properties, such as the force (or pressure) on

confining walls. This is because the entropic contribution to these free energies, and the associated forces is not naturally coming out of a typical simulation.

In collaboration with professor Eugene M. Terentjev from University of Cambridge (Cavendish Laboratory), we developed an alternative method, based on the empirical measurement of the average harmonic force that is needed to confine the chain, and from which we can reconstruct, in analytical way, the confinement free energy expression. Our first results show the correct contribution due to the pair excluded-volume interactions to the confinement free energy for a flexible self-avoiding chains, as predicted by the Flory theory. We are currently in the process of analyzing the latest results and writing a paper.

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Project title: Dynamical Masses and Gauge invariance: beyond the perturbative approach

Process Number: 2023/03722-9

Duration: 01/08/2023 to 31/07/2025

Period covered by Scientific Report: 01/08/2023 to 30/11/2023

Summary of the proposed project

Non-abelian Yang-Mills gauge theories describing the electroweak and strong interaction, cornerstones of the Standard Model, are far from completely understood. Perturbative Quantum Chromodynamics describes the high-energy region of the strong interaction successfully, but until today no coherent analytical description of the low-energy region exists. (Gauge-fixed) lattice results indicate massive behaviour of the gluon propagator in the low-energy regime. In the electroweak sector, spontaneous symmetry breaking of a "global gauge symmetry" is the only known way to provide masses for elementary vector bosons, but this is theoretically inconsistent and, even more disturbing, leads to explicit gauge dependence of the elementary Källén-Lehmann spectral functions. We construct analytical frameworks for gauge-invariant mass generation in Yang-Mills theories. Therefore we use local gauge-invariant composite operators in the Fröhlich-Morchio-Strocchi (FMS) framework to not only access the electroweak spectrum but also the phase structure in an explicitly gauge-invariant fashion. We will obtain gauge-invariant results predicting the results of Standard Model electroweak theory, as well as extend the description of massive gauge bosons to Minkowski spacetime. We test the Nielsen identities that guarantee gauge parameter independence (but not gauge invariance) of physical observables. We also study the deconfinement transition for pure Yang-Mills models at finite temperature with a dynamically generated mass while preserving the gauge symmetry.

Data management plan

Not applicable to this project, no data is being collected

Achievements in this period

In the period covered (01/08/2023 - 30/11/2023), I have started working on the topics described in the summary. In particular, I am collaborating with Prof. Gastao Krein (IFT-UNESP) on a project of massive gluons in Minkowski spacetime. In this project, we are working together with Prof. David Dudal (KU Leuven, Belgium), starting from the one-loop gluon propagator in Minkowski spacetime. For this, we have met with Prof. David Dudal in Rio de Janeiro for the period 05/11/2023 to 09/11/2023. I have also finished another project with Prof. Dudal in collaboration with Dr. Giovanni Peruzzo (UFF, Rio de Janeiro) and Prof. Silvio Sorella (UERJ, Rio de Janeiro) on BRST invariant scalar and vector operators in the $SU(2) \times U(1)$ Higgs model. This work uses the above described FMS framework in combination with the BRST-invariant extension of the Higgs field in the Stueckelberg formulation. This work was accepted THE EUROPEAN PHYSICAL JOURNAL C (Particles and Fields) and will be published shortly.

I also held several talks in the last few months:

- **11/10/2023:** IFT-UNESP, "Working towards a gauge-invariant description of the Higgs model: from local composite operators to spectral density functions".
- **27/10/2023:** LFTC UCS/UNICID, "Introduction to QCD"
- **08/11/2023:** Universidade Federal Fluminense, "Signatures of the Yang-Mills deconfinement transition from the gluon two-point correlator"

Activity plan for the next period

In the next period, I will continue my research in collaboration with Prof. Krein and also with Prof. Dudal. I am also involved as a co-supervisor of the Master Thesis of the student Wout Koeken at KU Leuven, in collaboration with Prof. Dudal, which will also continue in the next period. In the period 15/01/2024 to 04/03/2023, I will be teaching a summer course on QCD for Master students, together with Prof. Krein. The program and further information can be found on https://www.ift.unesp.br/Home/pesquisa/program_introqcd.pdf.

List of publications in the period covered by Scientific Report

D. Dudal, D.M. van Egmond, G. Peruzzo, S.P. Sorella, "BRST invariant scalar and vector operators in the $SU(2) \times U(1)$ Higgs model", e-Print: 2309.16776 [hep-th]. Accepted for publication by EUROPEAN PHYSICAL JOURNAL C.

Scientific Report

FAPESP

Post-doctoral Fellowship

Process: 2023/03917-4

Title: Synchronization of frustrated Kuramoto oscillators on modular networks

Beneficiary: Guilherme Henrique da Silva Costa

Advisor: Nathan Jacob Berkovits

Host institution: Instituto de Física Teórica/IFT/UNESP

Duration: 01/05/2023 to 30/04/2025

Report period: 01/05/2023 to 30/11/2023

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1 Project summary

The emergence of synchronization and its general features are of particular interest to scientists working on several fields, such as physics, social sciences and biology. From neurons to population dynamics and fireflies, nature showcases several examples of synchronized and collective behavior. In order to understand the basic properties leading to synchronization, Kuramoto proposed a model that became a paradigm in the field, being studied extensively in recent years.

The original model consists of N oscillators, described by internal phases θ_i , that rotate with natural frequencies ω_i , extracted from a given distribution. The oscillators are coupled according to the equations

$$\dot{\theta}_i = \omega_i + \frac{K}{N} \sum_{j=1}^N \sin(\theta_j - \theta_i), \quad (1)$$

where K is the coupling strength. Kuramoto analyzed this system in the $N \rightarrow \infty$ limit and showed that the system exhibited a second order (continuous) phase transition from disordered to synchronization as the control parameter K varies. For small values of K , the oscillators move as if they were independent, however, after a threshold K_c they started to cluster together, characterizing spontaneous synchronization.

Since the original publication of the model in 1975, several extensions and generalizations were proposed, such as replacing the all-to-all coupling to interactions with first neighbors on networks of different topologies, external forces acting on the oscillators, and higher dimensions. An interesting generalization recently involves changing the scalar coupling K to a matrix \mathbf{K} . The first investigations involving this model discovered novel behaviors during the synchronization transition, including active states and phase tuning, which are not found in the original Kuramoto model. However, the matrix coupling, namely frustrated Kuramoto model, was studied only in the context of all-to-all interactions. In real systems, the elements usually have an interacting neighborhood, that can be modeled as a network. Therefore, the study of this model on complex topologies, for example random or scale-free networks, is an interesting open subject that may bring out novel aspects and behaviors regarding synchronization phenomena.

A particular topology that draws attention to spreading and synchronization phenomena are the modular networks: a collection of nodes organized in groups with the property of being densely connected within the group but interacting weakly with vertices outside the module. Modular networks are interesting substrates to mimic community structure presented in real systems such as neuronal, social and biological networks. Considering the particular case of neuronal networks, another important factor is the effect of external forces driving the oscillators, since the synchronization and spreading of neurons signals are driven by an initial spiking acting on a small portion of neurons. Thus, inspired by the behavior of neuronal synchronization, we intend to study the frustrated Kuramoto model under the influence of external forces on modular networks.

2 Achievements

During the course of the project, our research questions remained within the original project, to investigate extensions and generalizations of the frustrated Kuramoto model, via matrix coupling, on modular substrates and under the influence of external forces. A mix between numerical analysis and analytical calculations were used to investigate several facets of this problem.

As a first approach to modular structures, we considered a complete graph of oscillators divided into two groups \mathcal{G}_1 and \mathcal{G}_2 . We have coupling matrices \mathbf{K}_1 and \mathbf{K}_2 describing the interactions within the groups and $\mathbf{K}_{12} = \mathbf{K}_{21}$ as the interactions between the two groups. By using the Ott-Antonsen ansatz, we were able to reduce the complexity of this problem to a set of four differential equations describing the order parameters of each group \mathcal{G}_i . Although the resulting equations were too complex for a general stability diagram, by investigating some particular cases, we could infer some interesting behaviors regarding the segregation (each module having their own dynamic) or integration (both modules acting as one entity) of the groups. In particular, for a given subset of parameters, we found a very complex diagram that describes the tug of war amongst modules to lead the dynamics of the system as a whole, including a region of complete desynchronization, indicating that the interactions between the groups can be destructive.

This first study was presented in an international conference named Conference on Complex Systems 2023 that occurred in Salvador-BA and is in the writing process of the article. We expect to submit the paper within the next few months. In other research branches, we started to collect and investigate the property of real modular networks, such as the *C. elegans* and *Drosophila* connectomes, outlining the best way to study the model on these substrates. Preliminary analyzes of the frustrated Kuramoto model in synthetic complex networks were also carried out, as well as the effect of external forces in a context of all-to-all interactions.

Invited talks

1. “Spreading dynamics in active matter models”, [ICTP-SAIFR Meetings on Soft and Biological Matter](#), IFT-UNESP, São Paulo, Brazil.

Journal reviewer

1. *Mathematical Biosciences and Engineering*, AIM Press.
2. *Journal of Physics: Complexity*, IOP Science.

Data management plan

The relevant data was published together with the works mentioned in Section 5 and/or can be found in the graphs and text of the manuscripts in the following sections.

The relevant data was published together with the works mentioned in Section 5 below and/or can be found in the graphs and text of the manuscripts in the sections below.

3 Activity plan for the next months

The following research activities are planned for the next months, in a probable order of execution:

1. Finalize and submit the manuscript regarding the dynamic of frustrated Kuramoto oscillators modularly connected.
2. Finalize the investigation into the effects of matrix coupling on Kuramoto oscillators in synthetic and real complex networks.
3. Write the article relating to the findings of item 2. Preliminary investigations indicate that the results are suitable for publication.
4. Complete the investigation into the effects of external driving forces on the matrix coupling Kuramoto oscillators.

In addition to the research, there are several important conferences where the studies developed in this project may be presented, such as the Autumn Meeting of the Brazilian Physics Society 2024 and the International School and Conference on Network Science, NetSci 2024.

4 Participation in scientific events

Presentations in conferences

1. **Event:** Conference on Complex Systems 2023, Salvador, Brazil, October 16-20, 2023
Poster presentation: “*Dynamic of frustrated Kuramoto oscillators with modular connections*”
Official note: “This work was presented by Guilherme S. Costa as an poster presentation at the scientific event Conference on Complex Systems 2023 held from October 16 to October 20, 2023, in Salvador, Brazil” using “**Reserva Técnica**” funds. In Portuguese for official completeness, this reads “Este trabalho foi apresentado por Guilherme S. Costa em formato de pôster no evento científico Conference on Complex Systems 2023 ocorrido de 16 a 20 de Outubro de 2023 em Salvador, Brasil” usando fundos da **Reserva Técnica**.
Event webpage: <https://ccs2023.org/>

Attendance of school

1. **Event:** Three-day event entitled *Brazilian Workshop on Soft Matter* at ICTP-SAIFR that consisted in several research seminars on Soft and Active Matter, in addition to a scientific visit in the new Brazilian synchrotron light source (Sirius).

Event webpage: <https://www.ictp-saifr.org/sm2023/>

5 List of publications

Publication 1 is a poster presented at a conference, where I investigated the segregation and integration dynamics of frustrated Kuramoto models divided into two groups. Following this section, the full publication can be found.

1. **Authors:** Guilherme S. Costa and Marcus A. M. de Aguiar

Title: “Dynamic of frustrated Kuramoto oscillators with modular connections”

Details: Presented at “Conference of Complex Systems 2023, Salvador, Brazil, October 16-20, 2023”

Open-access link: <http://dx.doi.org/10.13140/RG.2.2.35977.21606>

Dynamic of frustrated Kuramoto oscillators with modular connections

Guilherme S. Costa¹ and Marcus M. A. de Aguiar^{1,2}

¹ICTP South American Institute for Fundamental Research & Instituto de Física Teórica, Universidade Estadual Paulista - UNESP, São Paulo, Brazil

²Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas - Unicamp, Campinas, São Paulo, Brazil

guilherme.costa@ictp-saifr.org, aguiar@ifi.unicamp.br



Introduction

- The emergence of synchronization is of particular interest to scientists from several areas, such as physics, social sciences and biology. Kuramoto [1] proposed a model that became a paradigm in the field [2]. This model undergoes a second order phase transition from disordered motion to synchronization as the coupling between oscillators k increases.
- Several extensions of the original model were proposed, such as embedding the system on complex networks or interactions with external forces. A recent interesting one was to change the coupling from a scalar to a matrix, breaking the rotational symmetry and leading to generalized frustration [3].
- Modular topologies draws attention to synchronization phenomena for being substrates used to mimic community structure presented in real systems such as neuronal and biological networks.
- Based on that, we investigate analytically and numerically the dynamic of the matrix coupling Kuramoto model on a complete graph divided into two groups.

Methodology

Frustrated Kuramoto oscillators

- Dynamical equation:

$$\frac{d\vec{\sigma}_i}{dt} = \mathbf{W}_i \vec{\sigma}_i + \frac{1}{N} \sum_{j=1}^N [\mathbf{K} \vec{\sigma}_j - (\vec{\sigma}_i \cdot \mathbf{K} \vec{\sigma}_j) \vec{\sigma}_i], \quad (1)$$

- Natural frequencies:

$$\mathbf{W}_i = \begin{pmatrix} 0 & -\omega_i \\ \omega_i & 0 \end{pmatrix}.$$

- Parametrization of the coupling matrix:

$$\mathbf{K} = K \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} + J \begin{pmatrix} -\cos \beta & \sin \beta \\ \sin \beta & \cos \beta \end{pmatrix}.$$

- Order parameter:

$$\vec{p} = \frac{1}{N} \sum_i \vec{\sigma}_i = (p \cos \psi, p \sin \psi).$$

Ott-Antonsen (OA) ansatz

- $f(\omega, \theta, t) \rightarrow$ density of oscillators with natural frequency ω at position θ in time t .
- f satisfies the continuity equation $\frac{\partial f}{\partial t} + \frac{\partial(fv_\theta)}{\partial \theta} = 0$.
- OA ansatz [4]:** Coefficients of f Fourier expansion are chosen as $\rho^{(m)} e^{-im(\theta)}$.

$$f(\omega, \theta, t) = \frac{g(\omega)}{2\pi} \sum_{m=-\infty}^{\infty} \rho^{(m)} e^{im(\theta - \omega t)}. \quad (2)$$

- Useful for Lorentzian distributions $g(\omega) = \frac{1}{\pi} \frac{\Delta}{(\omega - \omega_0)^2 + \Delta^2}$.

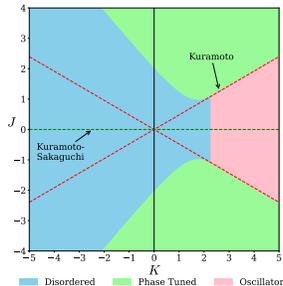


Fig. 1: Phase diagram on $K \times J$ space ($\alpha = 0.5, \beta = 0, \Delta = 1$ and $\omega_0 = 0$) for the frustrated Kuramoto model.

Modular connections

- As a first approach to modular structures, we considered a complete graph of oscillators divided into two groups M_1 and M_2 . Coupling matrices \mathbf{K}_1 and \mathbf{K}_2 describe the interactions within the group and $\mathbf{K}_{12} = \mathbf{K}_{21} = K_{12} \mathbf{1}$ the interactions between the groups.
- By applying the OA ansatz, we obtained four equations that describe the dynamic of the system:

$$\begin{aligned} \dot{p}_1 &= -\Delta_1 p_1 + \frac{p_1}{2} (1 - p_1^2) [K_1 \cos \alpha_1 - J_1 \cos(2\psi_1 + \beta_1)] + \frac{p_2}{2} (1 - p_1^2) K_{12} \cos \xi \\ \dot{p}_2 &= -\Delta_2 p_2 + \frac{p_2}{2} (1 - p_2^2) [K_2 \cos \alpha_2 - J_2 \cos(2\psi_2 + \beta_2)] + \frac{p_1}{2} (1 - p_2^2) K_{12} \cos \xi \\ p_1 \dot{\psi}_1 &= +\omega_1 p_1 - \frac{p_1}{2} (1 + p_1^2) [K_1 \sin \alpha_1 - J_1 \sin(2\psi_1 + \beta_1)] - \frac{p_2}{2} (1 + p_1^2) K_{12} \sin \xi \\ p_2 \dot{\psi}_2 &= +\omega_2 p_2 - \frac{p_2}{2} (1 + p_2^2) [K_2 \sin \alpha_2 - J_2 \sin(2\psi_2 + \beta_2)] + \frac{p_1}{2} (1 + p_2^2) K_{12} \sin \xi \end{aligned}$$

in which $\xi = \psi_1 - \psi_2$; \bar{p}_1 and \bar{p}_2 are order parameters for each module.

Results

Phase diagram for identical modules

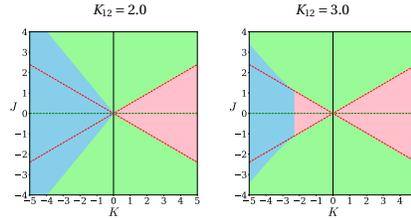


Fig. 2: Phase diagrams in the $K \times J$ space ($\alpha = 0.5, \beta = 0, \Delta = 1$ and $\omega_0 = 0$) for two identical modules. The value of K_{12} is shown above the respective graph. Colors are the same as in Fig. 1.

M_1 with $J = 0$; M_2 with $K = 0$

- Fixed parameters:** $K_1 = 10$; $J_2 = 3$; $\omega_1 = \omega_2 = 0$; $\Delta_1 = \Delta_2 = 1$
- Variables:** α and K_{12}

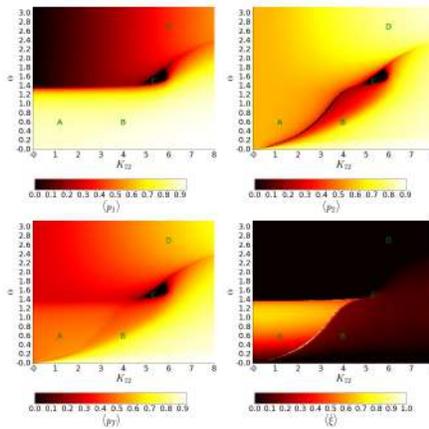
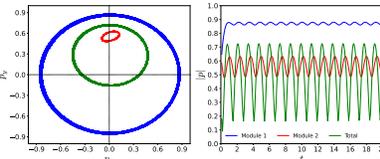
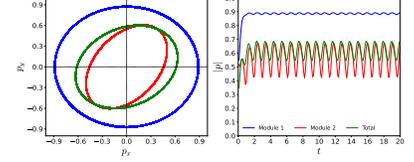


Fig. 3: Heatmaps in $\alpha \times K_{12}$ space showing time averages of some metrics. **Upper Left:** order parameter for M_1 (p_1); **Upper Right:** order parameter for M_2 (p_2); **Lower Left:** order parameter total (p) and **Lower Right:** difference of frequency ξ . A, B, C and D indicates points in which the dynamic of the system will be investigated.

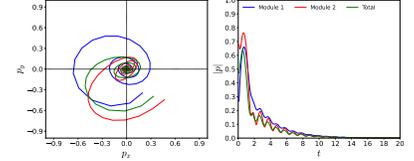
- A:** $\alpha = 0.6$ and $K_{12} = 1.20$



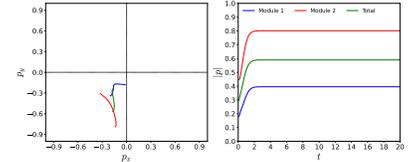
- B:** $\alpha = 0.6$ and $K_{12} = 4.00$



- C:** $\alpha = 1.5$ and $K_{12} = 5.35$



- D:** $\alpha = 2.7$ and $K_{12} = 6.00$



Discussions and Perspectives

- By applying the OA ansatz to a system with two modules totally connected, we reduced the complexity of the problem to four equations that describe the dynamic of the order parameter of the frustrated oscillators.
- Considering identical modules, the equations become simple enough to perform analytical analyses and $K \times J$ phase diagrams can be constructed. By increasing the intermodular coupling K_{12} , it becomes easier for the system to synchronize.
- Although the equations for distinct modules are complicated to analyze analytically, we performed numerical integrations considering M_1 with $J = 0$ and M_2 with $K = 0$ to investigate the joint dynamics of these modules.
- We found complex heatmaps on $\alpha \times K_{12}$ plane with distinct and rich behaviors of the modules. By inspecting some regions, we identified four outcomes for the modules dynamic:
 - Independent** \rightarrow The modules maintain their uncoupled dynamic.
 - Integrated oscillation** \rightarrow Both modules rotate at similar frequencies.
 - Phase tuned** \rightarrow The modules lock on a specific position of p -plane.
 - Disordered** \rightarrow The system unsynchronizes.
- As a perspective, we intend to investigate the frustrated Kuramoto model on real modular networks, assigning a distinct coupling matrix to each module.

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Formulário de Justificativa I de Aplicação dos Recursos da Reserva Técnica de Bolsas

Para processos com trâmite em papel - anexe UMA VIA ao RC enviado à FAPESP

Para processos SAGe - anexe o arquivo preenchido

PROCESSO: 2023/03917-4

Bolsista: Guilherme Henrique da Silva Costa

Orientador/Supervisor: Dr. Nathan Jacob Berkovits

 Declaro que não houve utilização dos Recursos da Reserva Técnica

JUSTIFICATIVA DAS DESPESAS REALIZADAS NA AQUISIÇÃO DE:

MATERIAL PERMANENTE

MATERIAL DE CONSUMO

SERVIÇOS DE TERCEIROS

Instruções para preenchimento

Justificar todas as despesas conforme as [normas da Reserva Técnica de Bolsa](#) disponíveis no portal da FAPESP na internet.

Para participação em eventos, utilize o formulário de Justificativa II.

Material Permanente: Justificar cada livro ou equipamento adquirido incluindo seus acessórios.

Material de Consumo: Agrupar os itens por justificativa de uso no projeto.

Serviços de Terceiros: Agrupar os itens por justificativa de uso no projeto. A nota fiscal ou recibo deve detalhar o serviço executado.

Tipo de despesa		Nº da Nota Fiscal/Recibo	
Justificativa de uso no projeto		Valor R\$	

Tipo de despesa		Nº da Nota Fiscal/Recibo	
Justificativa de uso no projeto		Valor R\$	

Tipo de despesa		Nº da Nota Fiscal/Recibo	
Justificativa de uso no projeto		Valor R\$	

Tipo de despesa		Nº da Nota Fiscal/Recibo	
Justificativa de uso no projeto		Valor R\$	

Formulário de Justificativa II de Aplicação dos Recursos da Reserva Técnica de Bolsas**Para processos com trâmite em papel - anexe UMA VIA ao RC enviado à FAPESP****Para processos SAGe - anexe o arquivo preenchido**

PROCESSO: 2023/03917-4

Bolsista: Guilherme Henrique da Silva Costa

Orientador/Supervisor: Dr. Nathan Jacob Berkovits

Justificativa das despesas realizadas com participação em evento

Tipo de Evento		Reunião Científica/Tecnológica (Congressos, Conferências, Seminários, Simpósios, Workshops/outros)			
Local	No País	Cidade/País	Salvador		
Início	16/10/2023	Término	20/10/2023	Duração (meses e dias)	5 dias
Título do Evento ou Instituição visitada		Conference on Complex Systems			
DESPESAS REALIZADAS	VALOR R\$				
Passagem Aérea	2.277,44				
Percurso / Observações	Ida: 15/10/2023 Congonhas/SP → Salvador/BA e volta: 21/10/2023 Salvador/BA → Guarulhos/SP				
Transporte Terrestre					
Percurso / Observações					
Taxa de Inscrição	706,16				
Seguro Saúde (no Exterior)					
Visto (no Exterior)					
Diária					
Manutenção (no Exterior)					
Total	2.983,60				

Resumo das atividades desenvolvidas

Apresentação de trabalho relacionado ao projeto, em formato painel, de nome: "Dynamic of frustrated Kuramoto oscillators with modular connections".

Relatório Científico

Nome: Walter Esteban Riquelme Chamblas

Título do projeto: Observando as condições iniciais do universo com levantamentos fotométricos.

Número do Processo FAPESP: 2023/07640-7

Período de vigência: 01/11/2023 to 31/10/2025

Período coberto pelo Relatório Científico em questão: Started in 01/11/2023

1) Project summary

Cosmological surveys have proven helpful when describing the properties of the universe. They have been able to constrain the nature of its constituents and test its evolution with high precision. A pending task for future surveys is to shed light on the universe's initial conditions.

The project aims to use data from photometric surveys, such as the Dark Energy Survey (DES) and the future Legacy Survey of Space and Time (LSST) at the Vera Rubin Observatory, to extract the properties of the initial conditions of the universe. Cosmic inflation predicts statistical properties for the initial seeds that could still live within the large-scale structures (LSS) we see today. Different inflation models suggest that the initial fluctuations could have a beyond Gaussian distribution. This property is known as Primordial non-Gaussianity (PNG).

We will use summary statistics, such as the correlation function, to measure the amount of Primordial non-Gaussianity imprinted in the galaxies we see today from DES and LSST. Observational systematics and uncertainties of the photometry of galaxies could impact the constraints of Primordial non-Gaussianity. The project also involves assessing the impact of different aspects of photometric data in this measurement.

2) Achievements during the current period

I have recently joined the LSST-DESC collaboration as a member of the Brazilian participation group. I am planning to join the Large-scale Structure working group. Within the working group, we are currently preparing a project proposal about measuring PNG using LSS from DESC, preparing the ground for the first data release of LSST.

In parallel, within the DES collaboration, I'm developing the pipeline to measure PNG using DES galaxies, particularly looking for a tailor-made selection of galaxies that improve the constraints on PNG. Besides that, I am also studying the effect of different observational systematics on the photometric uncertainty of galaxies and assessing the impact of such uncertainties in the clustering of galaxies.

3) Data management plan

Currently the developed codes are private until they are finished. It is expected that the pipeline for measuring PNG will be shared publicly in Github in the future.

4) Participation in scientific events

No participation in scientific events since the start of the fellowship.

5) Publications during the current period

No new publications in the current period.

6) Submitted works during the current period

No submitted works in the current period.

Relatório Científico

2.1) FOLHA DE ROSTO

Nome: Louis Legrand

Título do projeto: Explorando o setor escuro com correlação cruzada de lenteamento de CMB e levantamentos de galáxias.

Número do Processo FAPESP: 2023/08560-7

Período de vigência: 01/11/2023 to 30/06/2024

Período coberto pelo Relatório Científico em questão: Start in 01/11/2023

2.2) RESUMO DO PROJETO PROPOSTO

Upcoming galaxy and CMB surveys, including LSST and CMB-S4, are an unprecedented opportunity to explore the dark sector of the Universe. By mapping the distribution and shape of billions of galaxies, and by reconstruction the CMB gravitational lensing induced by large scale structures, these experiments offer complementary observables that shed light on the matter distribution and the growth of cosmic structures.

This research project aims to develop the cross correlation and joint analysis of the LSST galaxy survey with CMB experiments, such as CMB-S4. By leveraging the synergies between these probes, we can overcome systematic limitations and break parameter degeneracies, enabling optimal constraints on key parameters such as the equation of state of dark energy and the sum of neutrino masses.

2.3) REALIZAÇÕES NO PERÍODO

I have joined the LSST- DESC collaboration, as a member of the Brazilian participation group. I joined the group in charge of the Modelling and Combined Probes, and my first project was to include the CMB lensing into the covariance matrix for the likelihood analysis. This will allow to obtain joint constraints on cosmological models, combining galaxy clustering, galaxy weak lensing and CMB lensing.

In parallel, I am continuing to develop the CMB lensing analysis for the next generation of surveys, using the maximum likelihood estimators. This new estimator allows to maximise the signal to noise ratio of the reconstructed CMB lensing field.

In practice I am participating in testing and developing the TJPCov code

2.4) PLANO DE GESTÃO DE DADOS

The code I am developing as part of the DESC collaboration is available on GitHub: <https://github.com/LSSTDESC/TJPCov>

The code I am developing for the CMB lensing estimator is also available on GitHub: <https://github.com/NextGenCMB/delensalot>
<https://github.com/carronj/Lenslt>

3) PLANO DE ATIVIDADES PARA O PRÓXIMO PERÍODO

In the next period, I will continue to develop the analysis of the cross correlation between CMB lensing and galaxy surveys. I plan to forecast the constraints on some parameters of interest, such as the sum of the neutrino masses, obtained when combined LSST with CMB surveys.

4) PARTICIPAÇÃO EM EVENTO CIENTÍFICO

27/10/23: Colloquium at Instituto de Física, USP, Cosmology with gravitational lensing of the Cosmic Microwave Background

5) LISTA DAS PUBLICAÇÕES NO PERÍODO

Legrand, Louis, and Julien Carron. "Robust and Efficient CMB Lensing Power Spectrum from Polarization Surveys." *Physical Review D* 108, no. 10 (November 14, 2023): 103516. <https://doi.org/10.1103/PhysRevD.108.103516>.

Accepted for Publication:

Saha, Sayan, Louis Legrand, and Julien Carron. "Cluster Profiles from Beyond-the-QE CMB Lensing Mass Maps." *arXiv*, October 3, 2023. <https://doi.org/10.48550/arXiv.2307.11711>.

7) LISTA DOS TRABALHOS PREPARADOS OU SUBMETIDOS

Belkner, Sebastian, Julien Carron, Louis Legrand, Caterina Umiltà, Clem Pryke, Colin Bischoff, and for the CMB-S4 Collaboration. "CMB-S4: Iterative Internal Delensing and r Constraints." *arXiv*, October 11, 2023. <https://doi.org/10.48550/arXiv.2310.06729>.

Euclid Collaboration, B. Bose, P. Carrilho, M. Marinucci, C. Moretti, M. Pietroni, E. Carella, et al. "Euclid Preparation TBD. Modelling Spectroscopic Clustering on Mildly Nonlinear Scales in beyond- Λ CDM Models." *arXiv*, November 22, 2023. <https://doi.org/10.48550/arXiv.2311.13529>.

Euclid Collaboration, A. C. Deshpande, T. Kitching, A. Hall, M. L. Brown, N. Aghanim, L. Amendola, et al. "Euclid Preparation: XXVIII. Modelling of the Weak Lensing Angular Power Spectrum." *arXiv*, February 9, 2023. <https://doi.org/10.48550/arXiv.2302.04507>.

Euclid Collaboration, G. Jelic-Cizmek, F. Sorrenti, F. Lepori, C. Bonvin, S. Camera, F. J. Castander, et al. "Euclid Preparation. TBD. Impact of Magnification on Spectroscopic Galaxy Clustering." *arXiv*, November 6, 2023. <https://doi.org/10.48550/arXiv.2311.03168>.

Euclid Collaboration, G. F. Lesci, M. Sereno, M. Radovich, G. Castignani, L. Bisigello, F. Marulli, et al. "Euclid Preparation. TBD. Galaxy Colour Selections with Euclid and Ground Photometry for Cluster Weak-Lensing Analyses." *arXiv*, November 27, 2023. <https://doi.org/10.48550/arXiv.2311.16239>.

Euclid Collaboration, L. Leuzzi, M. Meneghetti, G. Angora, R. B. Metcalf, L. Moscardini, P. Rosati, et al. "Euclid Preparation TBD. Characterization of Convolutional Neural Networks for the Identification of Galaxy-Galaxy Strong Lensing Events." *arXiv*, July 17, 2023. <https://doi.org/10.48550/arXiv.2307.08736>.

Euclid Collaboration, A. Pezzotta, C. Moretti, M. Zennaro, A. Moradinezhad Dizgah, M. Crocce, E. Sefusatti, et al. "Euclid Preparation. TBD. Galaxy Power Spectrum Modelling in Real Space." *arXiv*, December 1, 2023. <https://doi.org/10.48550/arXiv.2312.00679>.

Euclid Collaboration, D. Sciotti, S. Gouyou Beauchamps, V. F. Cardone, S. Camera, I. Tutusaus, F. Lacasa, et al. "Euclid Preparation. TBD. Forecast Impact of Super-Sample Covariance on 3×2 pt Analysis with Euclid." *arXiv*, October 24, 2023. <https://doi.org/10.48550/arXiv.2310.15731>.

Euclid Collaboration, K. Tanidis, V. F. Cardone, M. Martinelli, I. Tutusaus, S. Camera, N. Aghanim, et al. "Euclid Preparation. TBD. The Effect of Linear Redshift-Space Distortions in Photometric Galaxy Clustering and Its Cross-Correlation with Cosmic Shear." *arXiv*, September 5, 2023. <https://doi.org/10.48550/arXiv.2309.00052>.

Frusciante, N., F. Pace, V. F. Cardone, S. Casas, I. Tutusaus, M. Ballardini, E. Bellini, et al. "Euclid: Constraining Linearly Scale-Independent Modifications of Gravity with the Spectroscopic and Photometric Primary Probes." arXiv, June 21, 2023. <https://doi.org/10.48550/arXiv.2306.12368>.

Scientific Report

FAPESP

Post-doctoral Fellowship

Process: 2022/13872-5

Title: Pattern formation in active matter and biology: bacterial mixtures and vegetation

Beneficiary: Pablo Souza de Castro Melo

Advisor: Nathan Jacob Berkovits

Host institution: Instituto de Física Teórica/IFT/UNESP

Duration: 12/01/2022 to 11/30/2024

Report period: 12/01/2022 to 11/30/2023

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1 Project summary

The emergence of complex biological functions depends on the spontaneous formation of spatiotemporal patterns between agents such as cells, plants, and animals. In the first part of this project, we will investigate the collective behavior of binary mixtures of bacterial cells and how they undergo cooperative or competitive pattern formation. We will focus on phenomena similar to so-called “motility-induced phase separation” found in collections of active (i.e., motile) particles like bacterial fluids, where persistent motion takes the role of “attractive forces” in generating agglomeration. It is known that, compared with systems of identical particles, the phenomenology of passive (i.e., nonmotile) mixtures is much richer. The study of bacterial mixtures is therefore of great relevance as different bacterial species and strains frequently coexist in Nature. This project aims to discover new features that appear only for mixtures, e.g., the slow approach to stationary segregation in crowded environments, for which there are no results. Our research questions will be answered via a combination of theoretical methods, simulations, and collaboration with experimentalists.

Initially, we will consider reciprocal mixtures where both types of bacteria have the same motility properties, i.e., the same self-propulsion speeds and reorientation rates. As found in Biology, we will consider the scenario where the motility properties of each type are affected reciprocally by the presence of the other type. These “quorum-sensing” interactions can be achieved and tuned in the lab by genetically modifying each type’s biochemical signaling; in doing so, their motility properties will depend on the concentration of highly-diffusive molecules produced exclusively by the other type. With this mechanism, it was shown that co-localization (or anti-localization) of the bacterial types emerges. Nonetheless, several questions remain open. One example is the environmental coupling that arises for bacterial mixtures compartmentalized in spatial niches. Another question is whether bacterial types, say, A and B, can regulate their motilities such that A moves at higher self-propulsion speed in the presence of B while B moves at lower self-propulsion speed in the presence of A, effectively leading to a phenomenon preliminarily dubbed “type chasing”. Finally, we will consider mixtures of bacteria with different motilities. Answering these questions will provide important steps towards avoiding the pathogenic formation of bacterial agglomerates found in medical contamination.

Secondly, we will investigate the minimal ecological requirements for the formation of vegetation patterns. Particularly, we will study the structural effects of rainfall spatial gradients (as at the border of deserts) and their seasonal temporal variability. These features are expected to generate the coexistence of distinct patterns. A similar behavior occurs during the phase separation of thermodynamic fluids, where abrupt environmental changes are known to generate secondary domains on a matrix of evolving primary structures. Later in the dynamics, all domains merge together as the system approaches thermodynamic equilibrium. For vegetation patterns, however, thermodynamic equilibrium is absent, meaning that primary and secondary “domains” coexist indefinitely. The implications of such primary-secondary domain coupling will be analyzed. Our results will be compared with image analysis from available satellite data.

This project is designed to bring outstanding advances to the lively fields of active matter and theoretical ecology. It involves a synergy of interests as well as theoretical and

experimental expertises. The proposal is physically relevant, viable, and presents great potential for applications.

2 Achievements

Our research questions remained well within the original plan. There have been only mild changes due to collaboration opportunities that emerged during the course of the project. This is reflected in our publications and work in progress developed during this report period between 12/01/2022 and 11/30/2023. In this period, there were 3 published papers, 1 paper submitted and 3 conference presentations (see Section 6). As initially planned, in this project we have been unravelling various distinct *effects of heterogeneity* on the motion-shaped patterns of biologically inspired systems of particles, mostly mixtures of moving organisms with different motilities. Such effects have been studied using simulations, field theories based on partial differential equations, and other kinds of kinetic theory modeling.

2.1 Main results reported in published/submitted papers

The papers that have been either published or at least submitted in the report period present the following main results.

- **Publication 1 in Section 6:** We developed a new lattice model to study moving organisms in crowded scenarios and how their resulting spatial distributions affect the spread of diseases and information. More specifically, we have calculated how the properties of organism clustering induced by persistent movement, such as number of clusters, distance between clusters, sizes of clusters, etc., affect the final outcome of the spreading process. We found an intricate non-monotonic dependence between self-propulsion reorientation rate and the final size of the epidemics. Among other things, this new line of study is relevant in the context of phage therapy, where viruses are deliberately employed to spread in and kill bacterial colonies.
- **Publication 2 in Section 6:** We created a model for a mixture of fast and slow self-propelled (or “active”) particles, akin to a heterogeneous population of moving bacteria, in the presence of hard surfaces. Using simulations and a new analytical theory, we identified and explained a two-stage pattern formation in which bacteria accumulate on walls due to persistent movement. Patterns of spatial segregation between fast and slow particles evolve over long timescales due to particle crowding. This research can lead to new ideas to prevent the initiation of *biofilms*, that is, agglomerates of microorganisms that contaminate surfaces of medical instruments and organs.
- **Publication 3 in Section 6:** We studied the interaction between a mixture of slow and fast bacteria and an array of asymmetric obstacles. We found that this interaction generates particle vortices at obstacle corners, particle accumulation on obstacle surfaces, non-trivial spatial segregation between fast and slow particles, and

motion rectification, that is, the emergence of a nonzero transport current due to a coupling between obstacle asymmetry and movement persistence. We elucidated the origins of those behaviors.

- **Submitted work 1 in Section 7:** We devised a new spatial ecology model for individuals moving in a certain class of spatially heterogeneous environments. In particular, we studied critical habitat sizes, that is, the minimal size for the habitat of a biological population below which they go extinct. This topic is relevant in the context of deforestation and conservation biology. Spatial heterogeneity was introduced in two ways. First, there is a preferred location toward which individuals tend to *advect* (i.e., flow), on top of their Brownian-like movement. Second, there are good and harsh environment regions, defined in terms of different effective reproduction rates. We have found that, in certain regions of the space of parameters, advection may be detrimental to survival if the preferred location is close to the borders between good and harsh environments. We found how critical habitat properties depend non-monotonically on movement properties and provided new insights into the spatial population dynamics.

2.2 Work in progress

There is a number of other works in progress where significant advances have been made. The most important points are summarized below.

- **Spatial population dynamics with individual home-range creation.** We have developed a new model for the ecology of moving organisms where each individual has its own preferred location (home range center) toward which its diffusive movement is biased. This is called individual home range and corresponds to the behavior of several partially solitary species such as gorillas and jaguars. Understanding the consequences of individual-home-range movement to spatial ecology, where birth and death by competition are important, is an open problem. Here, we have created the first field theory that is able to combine individual home ranges and the birth of new individuals with new home range centers. The resulting integro-differential partial differential equation has been analyzed numerically and in terms of linear stability analysis of the initial conditions. Depending on the rules that determine the choice of a new home range center, distinct patterns in space have been found. We are now considering other types home-range establishment rules that depend on the current spatial distribution. We aim to identify more general properties of the emerging patterns and study how critical habitat properties change due to individual home ranges.
- **Spatial population dynamics of confined chemotactic individuals near toxic sources.** In collaboration with students supervised in the 2023 Quantitative Ecology program at ICTP-SAIFR, we have developed a field theory to study the spatial distribution and ecological persistence of confined populations that move (and die) in response to a toxic point source. This is important for the study of populations

in polluted confined environments such as lakes as well as for the design of new antibiotics. We found that population survival depends on a delicate balance provided by growth and toxic consumption which may be broken depending on the toxic injection site. Given enough time, a slowly-degrading toxic substance with lower diffusivity will kill more effectively. There exists an optimal value for toxic diffusivity that exterminates the population in a faster way. A paper on our findings is being written.

- **Transitions in optimal chemotactic foraging strategies in scarce scenarios.** We have studied single-particle systems of individuals undergoing random searches guided by smell cues emitted by a pattern of targets (vegetation patches, food, mates, etc.). We calculated the corresponding optimal random motion parameters toward which some species may have evolved, as hinted by experiments with bees and deer. Without scent, the optimal strategy is a power-law distribution of step sizes that mixes long and short steps. At intermediate scent spread length, however, we found that a discontinuous transition occurs, over which the optimal strategy becomes completely Brownian since large steps would risk placing the searcher too far from where the scent is useful. At even higher scent spread length, a second discontinuous transition occurs, now “backwards”: the scent profile becomes so flat that, despite far reaching, it cannot be useful. Our results shine a light on how the degree of external information sampling changes optimal foraging strategies for searchers in scarce environments. An intricate analytical theory is being carefully developed to support our findings.
- **Miscellaneous:** Besides the more advanced works discussed above, there are a number of significantly advanced projects in the field of Active Matter that are underway in collaboration with Danilo Liarte, Guilherme Costa and Márcio Gomes Sampaio (all from ICTP-SAIFR) as well as with Rodrigo Soto (Universidad de Chile), José Freire (UFPR), Felipe Hawthorne (USP), and Peter Sollich (University of Göttingen). These projects include studying the effects of other types of disease spread in spatial distributions of active entities, the movement of microorganisms in elastic networks such as collagen, and mixtures of active particles with quorum-sensing interactions. Finally, there are other more incipient collaborations that can be discussed in the future.

2.3 Other achievements

I participated and/or presented in a number of conferences and events. Other points are to be highlighted below, namely the organization of the Brazilian Workshop on Soft Matter at ICTP-SAIFR, participation as supervisor in a five-week project within the Quantitative Ecology program as well as invited talks and work as reviewer for a couple of journals.

Invited talks

1. Colloquium at University of Göttingen, “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”, Institute for Theoretical Physics, University of Göttingen, Germany.
2. Colloquium at Center for Advanced Systems Understanding, “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”, CASUS, Görlitz, Germany.
3. Colloquium at IFT-UNESP, “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”, São Paulo State University (UNESP), São Paulo, Brazil.
4. Seminar at IFT-UNESP, “Simple Models in Active Matter”, São Paulo State University (UNESP), São Paulo, Brazil.
5. Colloquium at IF-USP, “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”, São Paulo University (USP), São Paulo, Brazil.
6. Postgraduate Students Colloquium at IFT-UNESP, “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”, São Paulo State University (UNESP), São Paulo, Brazil.

Scientific event organizer

1. **Event:** Brazilian Workshop on Soft Matter, October 4-6, 2023 São Paulo, Brazil ICTP-SAIFR/IFT-UNESP & SIRIUS/CNPEM.
Role: Scientific organizer
Event link: <https://www.ictp-saifr.org/sm2023/>.

Journal reviewer

Below is a list of the journals where manuscripts were reviewed by the scholarship holder during the report period.

1. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, American Institute of Physics.
2. *PLOS Computational Biology*, PLOS.
3. *Soft Matter*, Royal Society of Chemistry.

Supervision

1. **Activity:** Supervision of hands-on five-week project within Quantitative Ecology program at ICTP-SAIFR, January-February 2023.
Role: Advisor of students group.
Project title: “Population spatial dynamics near toxic sources: a race for survival”.
Final presentation link: shorturl.at/qFHKR.
Program link: www.ictp-saifr.org/qecoprogram/.

2.4 FAPESP Career Consolidation Program

1. The scholarship holder participated in the “Programa Iniciativa de Mentoria para Consolidação da Carreira em Pesquisa dos bolsistas de Pós-Doutorado (PD) da FAPESP”, 12-14 April 2023. Program link: <https://mentoriapd.fapesp.br>.

3 Data management plan

The relevant data was published together with the works mentioned in Section 6 below and/or can be found in the graphs and text of the manuscripts in the sections below. On top of that, there is a link for relevant codes on the “How movement bias to attractive regions determines population spread and critical habitat size” manuscript: <https://github.com/VivianDornelas/SpatialPopulationModeling>.

4 Plan of activities for the next period

1. **Presentation and Supervision in the Summer School for Young Physicists at ICTP-SAIFR, 15-20 January 2024.** The scholarship holder will give a presentation and supervise a one-week hands-on project on the Physics of Complex Systems, including Active Matter and the Collective Movement of Organisms. Program link: <https://outreach.ictp-saifr.org/escolaverao/>.
2. **Scientific Session Organization.** In the APS/SAIFR Satellite March Meeting March 3-8, 2024, the scholarship holder will organize a session on Complex Systems and Soft Matter.
3. **School and Workshop Organization.** The scholarship holder will act as main scientific coordinator of a School and Workshop on Active Matter at ICTP-SAIFR between 30 September and 4 October 2024. This event has been already approved by the Institute. The school will have the following confirmed lecturers:
 - Julia Yeomans, University of Oxford, on *Active nematics and tissues*
 - Rodrigo Soto, Universidad de Chile, on *Kinetic Models of Active Suspensions*
 - Peter Sollich, University of Göttingen, on *Phase behavior and glassy dynamics*

4. **Research and Publications.** There are three advanced works which will be concluded and submitted in 2024. Their main results so far are discussed in the “Work in progress” section above. On top of that, we will continue with additional new research as discussed in the last point (“Miscellaneous”) of the “Work in progress” section.
5. **Participation in Scientific Events.** The scholarship holder aims to participate in several conferences as listed below.
 - “Encontro de Outono”, Brazilian Physical Society, EOSBF 2024, scheduled to be held in Florianópolis, Santa Catarina.
 - School on Biological Physics across Scales: Pattern Formation November 11-22, 2024, ICTP-SAIFR
 - One conference in Europe or in the United States. Yet to be decided. Possibilities: 1. The Many Faces of Active Mechanics, October 15-18, 2024, Boulder, USA; 2. Liquid Matter Conference 2024, 22-27 September, Mainz, Germany.

5 Participation in scientific events in the report period

Presentations in conferences

Only some of the conferences have used funds from the “Reserva Técnica”. More details are given below. The slides and poster of the corresponding presentations can be found at the end of Section [6](#).

1. **Event:** Encontro de Outono da SBF, Ouro Preto, Minas Gerais, Brazil, 21-25 Maio 2023.
Oral presentation: “*Spatial Distribution of Confined Interacting Organisms*”, *Brazilian Physical Society*
Event webpage: www1.fisica.org.br/eosbf/2023/index.php/en/
Official note: “This work was presented by Pablo de Castro as an oral presentation at the scientific event Encontro de Outono da SBF, Ouro Preto, Minas Gerais, Brazil, 2023” using “Reserva Técnica” funds. In Portuguese for official completeness, this reads as follows: “Este trabalho foi apresentado por Pablo de Castro como apresentação oral no evento científico Encontro de Outono da SBF, Ouro Preto, Minas Gerais, Brasil, 2023” utilizando recursos da “Reserva Técnica”.
2. **Event:** Active Matter at Surfaces and in Complex Environments, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, 19 - 23 June 2023.
Poster presentation: “*Mixtures of active Brownian particles interacting with walls and obstacles*”
Event webpage: www.pks.mpg.de/amsce23
Official note: “This work was presented by Pablo de Castro as an oral presentation at the scientific event *Active Matter at Surfaces and in Complex Environments*,

Max Planck Institute for the Physics of Complex Systems, Dresden, Germany” using “**Reserva Técnica**” funds. In Portuguese for official completeness, this reads as follows: “Este trabalho foi apresentado por Pablo de Castro como apresentação oral no evento científico *Active Matter at Surfaces and in Complex Environments*, Max Planck Institute for the Physics of Complex Systems, Dresden, Alemanha” usando fundos da **Reserva Técnica**.

3. **Event:** ICTP School on Collective Animal Behaviour, La Havana, Cuba, November 13-24, 2023
Oral presentation: “*Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers*”
Event webpage: <https://indico.ictp.it/event/10226>

Attendance of school

1. **Event:** ICTP School on Collective Animal Behaviour, La Havana, Cuba, November 13-24, 2023.
Event webpage: <https://indico.ictp.it/event/10226>

6 List of Publications in the Report Period

Copies of the following works can be found at the end of this document. As recommended, oral and poster presentations at conferences are also listed.

6.1 Papers

1. **Authors:** Pablo de Castro, Felipe Urbina, Ariel Norambuena, and Francisca Guzmán-Lastra
Title: “Sequential epidemic-like spread between agglomerates of self-propelled agents in one dimension”
Journal and number: *Physical Review E*, 108, 044104, 2023.
DOI: 10.1103/PhysRevE.108.044104
2. **Authors:** Mauricio Rojas-Vega, Pablo de Castro, and Rodrigo Soto
Title: “Wetting dynamics by mixtures of fast and slow self-propelled particles”
Journal and number: *Physical Review E*, 107, 014608, 2023.
DOI: 10.1103/PhysRevE.107.014608
3. **Authors:** Mauricio Rojas-Vega, Pablo de Castro, and Rodrigo Soto
Title: “Mixtures of self-propelled particles interacting with asymmetric obstacles”
Journal and number: *The European Physical Journal E*, 46, 95, 2023.
DOI: 10.1140/epje/s10189-023-00354-y

6.2 Conference presentations

1. **Authors:** Pablo de Castro
Title: “Spatial Distribution of Confined Interacting Organisms”, Brazilian Physical Society”
Details: Oral presentation given at Encontro de Outono da SBF, Ouro Preto, Minas Gerais, Brazil, 21-25 Maio 2023
Open-access link: <https://rb.gy/6l50wg>
2. **Authors:** Pablo de Castro
Title: “Collective Dynamics of Moving Organisms: The Statistical Physics of Self-Propelled Random Walkers”
Details: Oral presentation given at the ICTP School on Collective Animal Behaviour, La Havana, Cuba, November, 13-24, 2023
Open-access link: <https://rb.gy/233w02>
3. **Authors:** Pablo de Castro, Mauricio Rojas-Vega, and Rodrigo Soto
Title: “Mixtures of active Brownian particles interacting with walls and obstacles”
Details: Poster presented at “Active Matter at Surfaces and in Complex Environments”, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, 19 - 23 June 2023.
Open-access link: <https://rb.gy/26po6l>

Sequential epidemic-like spread between agglomerates of self-propelled agents in one dimensionPablo de Castro ^{*}*ICTP-South American Institute for Fundamental Research - Instituto de Física Teórica da UNESP,
Rua Dr. Bento Teobaldo Ferraz 271, 01140-070 São Paulo, Brazil*Felipe Urbina and Ariel Norambuena *Centro Multidisciplinario de Física, Universidad Mayor, Huechuraba, 8580745 Santiago, Chile*Francisca Guzmán-Lastra *Department of Physics, Faculty of Sciences, Universidad de Chile, 7830030 Santiago, Chile*

(Received 30 March 2023; accepted 13 September 2023; published 2 October 2023)

Motile organisms can form stable agglomerates such as cities or colonies. In the outbreak of a highly contagious disease, the control of large-scale epidemic spread depends on factors like the number and size of agglomerates, travel rate between them, and disease recovery rate. While the emergence of agglomerates permits early interventions, it also explains longer real epidemics. In this work, we study the spread of susceptible-infected-recovered (SIR) epidemics (or any sort of information exchange by contact) in one-dimensional spatially structured systems. By working in one dimension, we establish a necessary foundation for future investigation in higher dimensions and mimic micro-organisms in narrow channels. We employ a model of self-propelled particles which spontaneously form multiple clusters. For a lower rate of stochastic reorientation, particles have a higher tendency to agglomerate and therefore the clusters become larger and less numerous. We examine the time evolution averaged over many epidemics and how it is affected by the existence of clusters through the eventual recovery of infected particles before reaching new clusters. New terms appear in the SIR differential equations in the last epidemic stages. We show how the final number of ever-infected individuals depends nontrivially on single-individual parameters. In particular, the number of ever-infected individuals first increases with the reorientation rate since particles escape sooner from clusters and spread the disease. For higher reorientation rate, travel between clusters becomes too diffusive and the clusters too small, decreasing the number of ever-infected individuals.

DOI: [10.1103/PhysRevE.108.044104](https://doi.org/10.1103/PhysRevE.108.044104)**I. INTRODUCTION**

The transmission of states through contact between individuals is a widespread phenomenon observed in various organisms such as animals [1–4], insects [5,6], micro-organisms [7], and other sorts of agents [8–10]. In movement epidemiology, a central problem is how individual spatial motion can influence transmission contact by changing encounter rates [11–13], therefore affecting epidemic spread [14,15]. Scenarios where individuals are not homogeneously distributed in space are particularly challenging [16]. For instance, motile organisms may form stable agglomerates such as cities or colonies. In fact, the occurrence of diseases typically happens in spatial clusters and then propagates between them. As a result, if one can anticipate further spreading, containment becomes feasible [17]. The existence of a spatial hierarchy of measles transmission in England and Wales was demonstrated through the study of population patches arranged in a line [18]. A more sophisticated version of this technique illustrates that excess human mortality related to

pneumonia and influenza in the United States is consistent with human travel patterns [19]. In the presence of clustering, epidemic spread should be controlled by the typical size of the agglomerates, their typical distance to one another, the rate at which individuals travel between them, and the disease recovery rate. Exactly how these quantities control epidemic spread is an understudied subject. We take the liberty to use the word “epidemic” throughout the text for representing any sort of transmission of a state between individuals or information exchange by contact, including diseases, short-range molecule signaling between micro-organisms or ants [20], and social consensus [8].

Increasing attention has been paid to models of self-propelled particles where epidemic spread emerges from individual motion rules [21–27]. One example is the active Brownian particle (ABP) model, where the particle moves with a self-propulsion velocity of constant magnitude and whose direction fluctuates stochastically and continuously [28–32]. This model has been largely used to model animal movement, particularly bacteria [31]. ABPs can spontaneously agglomerate into clusters even if subject to purely repulsive short-range interactions [33]. Such motility-induced clustering arises as particles block each other due to low

^{*}pablo.castro@ictp-saifr.org

Wetting dynamics by mixtures of fast and slow self-propelled particles

Mauricio Rojas-Vega,¹ Pablo de Castro^{2,*} and Rodrigo Soto³

¹*Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria*

²*ICTP South American Institute for Fundamental Research & Instituto de Física Teórica, Universidade Estadual Paulista - UNESP, 01140-070 São Paulo, Brazil*

³*Departamento de Física, FCFM, Universidad de Chile, Avenida Blanco Encalada 2008, Santiago, Chile*



(Received 1 September 2022; accepted 6 January 2023; published 24 January 2023)

We study active surface wetting using a minimal model of bacteria that takes into account the intrinsic motility diversity of living matter. A mixture of “fast” and “slow” self-propelled Brownian particles is considered in the presence of a wall. The evolution of the wetting layer thickness shows an overshoot before stationarity and its composition evolves in two stages, equilibrating after a slow elimination of excess particles. Nonmonotonic evolutions are shown to arise from delayed avalanches towards the dilute phase combined with the emergence of a transient particle front.

DOI: [10.1103/PhysRevE.107.014608](https://doi.org/10.1103/PhysRevE.107.014608)

I. INTRODUCTION

Natural active matter, such as collections of organisms, is *not* composed of identical self-propelling agents [1]. Instead, a wide distribution of motility properties exists due to different ages, reproduction stages, shapes, and sizes [2–4]. Moreover, active particles typically interact with “surfaces,” e.g., bacteria swimming near the boundaries of their host body or of contaminated medical instruments [5,6]. For simplicity, models usually ignore at least one of these two ingredients, i.e., diversity and surface effects.

A persistent particle has a self-propulsion direction that fluctuates stochastically and, typically, slowly [7]. Consequently, active matter accumulates on surfaces to an extent dependent on persistence and density [8]. For bacteria, this mechanism, together with other factors, contributes to initiate biofilm formation [9]. Surface accumulation by persistence is called active wetting [10–13]. Three phases are possible [8]: complete wetting, where the wetting layer covers the wall completely; incomplete wetting, where only a fraction of the wall becomes covered; and “unwetting” or “drying,” where no dense phase exists. Active wetting was studied mostly for identical particles. However, passive and active phase behaviors can depend strongly on “diversity” in some particle attribute [14–29].

In this paper, we study a mixture of “fast” and “slow” active Brownian disks moving in two dimensions (2D), in the presence of a flat impenetrable wall. Each type has its own self-propulsion speed, defining a degree of *speed diversity*. Besides simulations, a dynamical kinetic theory is developed by extending the approach of Redner *et al.* [30] in three fronts: to mixtures, to include walls, and to incorporate time dependence. This approach calculates the absorption and emission rates for the agglomerate directly from microscopic

considerations and is therefore different than free-energy-like approximations [31] or phenomenological theories [32] that can be harder to connect with microscopic properties. Our theory relies on one fitting parameter only (similarly to Redner’s original theory [30]), which assumes a single value across all parameters, somewhat as a “universal constant.” To isolate surface effects, we choose a range of densities that allows for significant complete wetting while bulk motility-induced phase separation (MIPS) remains absent. Instead of focusing on “equilibrium” wetting-drying transitions [8], we study the wetting dynamics, i.e., the mechanisms involved in setting the composition and thickness of the wetting layer versus time and how motility diversity affects those. A two-stage evolution is found. Moreover, we identify a transient overshoot of the layer thickness, which occurs even without diversity but whose intensity depends nonmonotonically on it.

II. MODEL AND SIMULATION METHOD

We consider a binary mixture in 2D composed of N active Brownian disks (labeled by i) where $N/2$ of them are “fast” particles, with self-propulsion speed $v_i = v_f \equiv v_0(1 + \delta)$, and the other $N/2$ are “slow” particles, with $v_i = v_s \equiv v_0(1 - \delta)$. Thus $\delta \in [0, 1]$ is the degree of speed diversity [33]. Hereafter “f” and “s” denote “fast” and “slow” particles, respectively. Their dynamics obeys

$$\partial_t \mathbf{r}_i = v_i \hat{\mathbf{v}}_i + \mu \mathbf{F}_i + \boldsymbol{\xi}_i, \quad \partial_t \theta_i = \eta_i(t), \quad (1)$$

where $\hat{\mathbf{v}}_i = (\cos \theta_i, \sin \theta_i)$ is the self-propulsion direction, μ is the mobility, and $\mathbf{F}_i = \sum_j \mathbf{F}_{ij} + \mathbf{F}_i^{\text{wall}}$ is the net force on particle i due to interactions with other particles and with the wall. The noise terms $\boldsymbol{\xi}_i(t)$ and $\eta_i(t)$ are Gaussian and white, with zero mean and correlations $\langle \xi_{i\alpha}(t) \xi_{j\beta}(t') \rangle = 2\xi \delta_{ij} \delta_{\alpha\beta} \delta(t - t')$ (the greek letters denote coordinates) and $\langle \eta_i(t) \eta_j(t') \rangle = 2\eta \delta_{ij} \delta(t - t')$, where ξ and η

*Corresponding author: pablo.castro@ictp-saifr.org



Mixtures of self-propelled particles interacting with asymmetric obstacles

Mauricio Rojas-Vega¹, Pablo de Castro^{2,a} , and Rodrigo Soto³

¹ Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

² ICTP South American Institute for Fundamental Research and Instituto de Física Teórica, Universidade Estadual Paulista - UNESP, São Paulo 01140-070, Brazil

³ Departamento de Física, FCFM, Universidad de Chile, Avenida Blanco Encalada 2008, Santiago, Chile

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Abstract In the presence of an obstacle, active particles condensate into a surface “wetting” layer due to persistent motion. If the obstacle is asymmetric, a rectification current arises in addition to wetting. Asymmetric geometries are therefore commonly used to concentrate microorganisms like bacteria and sperms. However, most studies neglect the fact that biological active matter is diverse, composed of individuals with distinct self-propulsions. Using simulations, we study a mixture of “fast” and “slow” active Brownian disks in two dimensions interacting with large half-disk obstacles. With this prototypical obstacle geometry, we analyze how the stationary collective behavior depends on the degree of self-propulsion “diversity,” defined as proportional to the difference between the self-propulsion speeds, while keeping the average self-propulsion speed fixed. A wetting layer rich in fast particles arises. The rectification current is amplified by speed diversity due to a superlinear dependence of rectification on self-propulsion speed, which arises from cooperative effects. Thus, the total rectification current cannot be obtained from an effective one-component active fluid with the same average self-propulsion speed, highlighting the importance of considering diversity in active matter.

1 Introduction

Active particles—such as bacteria, tissue cells, and autophoretic colloids—spontaneously accumulate on the surfaces of obstacles even in the absence of attractive forces [1, 2]. Similarly to motility-induced phase separation (MIPS) [3], such *active wetting* [4] arises when active particles have a direction of motion that evolves stochastically but slowly, i.e., their direction of motion is *persistent* [5–8]. For sufficiently large persistence times or densities, particles do not have time to find an escape route and thus become trapped between obstacles and other particles. Active wetting helps control surface adhesion and capillary properties of bacterial biofilms [9–11], whose formation makes bacterial colonies more resilient against antibiotics [12].

In the case of *asymmetric* obstacles, simulations and experiments show that active particles undergo directed motion [13], in addition to wetting [14]. The spontaneous emergence of net particle transport due to environmental asymmetries, i.e., rectification currents, has constituted a central topic in both conceptual and technological contexts for decades [15]. More recently, research on rectification of self-propelled particles has

gained momentum [16–27]. In Ref. [28], an initially homogeneous collection of active Brownian particles in 2D was simulated in a regular array of half-disk rigid obstacles. Each obstacle was oriented along the same fixed direction as the others. The stationary average velocity, computed over all particles of the system, was found to be nonzero. Instead, an effective rectification current emerges since particles traveling from the curved to the flat side of the obstacle spend less time trapped by the obstacle than those in the opposite direction.

Ref. [28] considered identical active particles, i.e., particles with the same self-propulsion speed, rotational diffusion coefficient, and size. However, in natural colonies of bacteria and other microorganisms, a broad dispersion of motility parameters exists due to different ages, reproduction stages, shapes, sizes, and running modes [29–32]. For either passive or active fluids, it is known that “polydispersity” or “diversity” of some particle attribute generates several new collective behaviors, including changing the nature and loci of phase diagram boundaries and introducing particle-type spatial segregation [6, 33–57]. Still, it remains unclear what is the extent to which particle diversity affects rectification in active matter, as well as what are the mechanisms behind potential effects of particle diversity. A

^a e-mail: pablo.castro@ictp-saifr.org (corresponding author)



Spatial distribution of confined interacting organisms

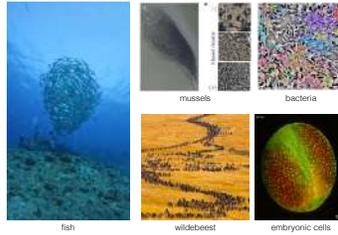
Pablo de Castro
ICTP-SAIFR
IFT-UNESP



Pablo de Castro

Active Matter & Spatial Ecology

We see patterns in collections of living organisms **across scales**



Pablo de Castro

Active Matter & Spatial Ecology

The Physics Approach



spherical cows

What are the equations of motion of living organisms?

What is the spatial distribution of living organisms?

How can interactions among organisms and the environment change their distribution?

Part 1: Active Matter
Part 2: Spatial Ecology

Pablo de Castro

Active Matter & Spatial Ecology

Active Matter

The Free Self-Propelled Particle



Example: *E. coli* bacteria



Active Brownian particle

$$\mathbf{r} = v(\cos \theta, \sin \theta)$$

$$\dot{\theta} = \eta_k$$

Equation of motion

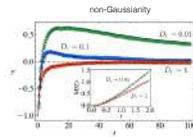


$v = 0.2\mu\text{m/s}$ $v = 1.2\mu\text{m/s}$ $v = 2.2\mu\text{m/s}$ $v = 3.2\mu\text{m/s}$

Pablo de Castro

Active Matter & Spatial Ecology

Truly **Gaussian** diffusion takes even longer!



$\text{MSD} \sim t$
is not enough!

Diffusion equation
cannot be used!

Andrea Villa-Sorrealba, Cristóbal Chávez-Ribay, Pablo de Castro & Rodrigo Soto

Phys. Rev. E 101, 062607

Pablo de Castro

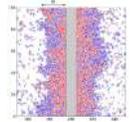
Active Matter & Spatial Ecology

Formation of accumulation layer by active mixtures
on boundaries is **non-monotonic** in time



Mechanism of **motility-induced phase separation**
for mixtures in the presence of walls

Motivation: biofilm initiation &
biological matter is diverse



Mauricio Rojas-Vega, Pablo de Castro & Rodrigo Soto

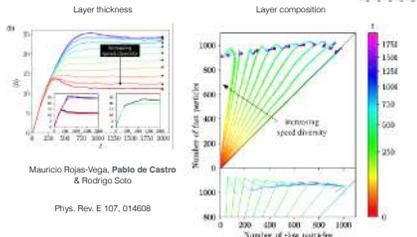
Phys. Rev. E 107, 014608

Pablo de Castro

Active Matter & Spatial Ecology

Formation of accumulation layer by active mixtures
on boundaries is **non-monotonic** in time

red: free speed = 1.0
blue: free speed = 0.2

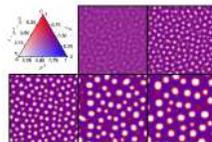


Mauricio Rojas-Vega, Pablo de Castro & Rodrigo Soto
Phys. Rev. E 107, 014608

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Active Matter & Spatial Ecology

Passive mixture phase separation is **also two-stage**
via **energetic** mechanism



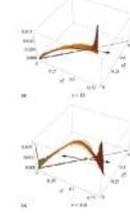
Pablo de Castro & Peter Sollich

Phys. Chem. Chem. Phys., 2017, 19, 22509-22527

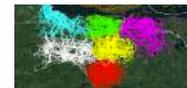
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Active Matter & Spatial Ecology

Histogram of compositions at different times



Spatial Ecology



Wolves GPS tracking data



Reproduction and competition are important

Large spatial scales and time scales

No accumulation by contact

Normal diffusion can be used

Ecological processes become relevant

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Active Matter & Spatial Ecology

Critical Habitat Size

Deforestation

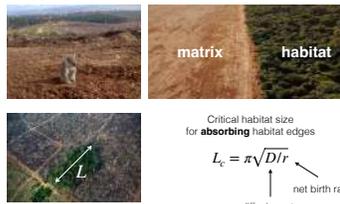


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Ecological Scale & Critical Habitat Size

Deforestation



Critical habitat size for absorbing habitat edges

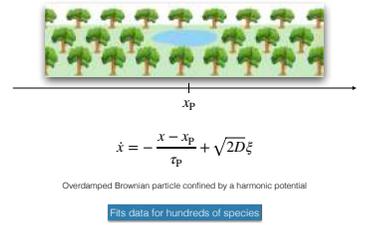
$$L_c = \pi \sqrt{D/r}$$

↑ net birth rate
diffusion rate

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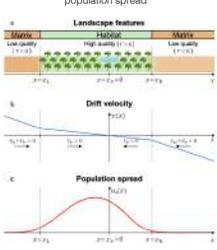
Attractive location: Range residency



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Active Matter & Spatial Ecology

Effect of attractive location on population spread



Death not instantaneous: **Movement-bias** avoidance of low-quality regions

$$\dot{x} = v_p(x) + v_M(x) + \sqrt{2D}\xi$$

$$v_p(x) = -\frac{x - x_p}{\tau_p}$$

$$v_M(x) = \begin{cases} \frac{x - x_M}{\tau_M} & \text{for } x \text{ in the left matrix} \\ 0 & \text{for } x \text{ in the habitat} \\ \frac{x - x_M}{\tau_M} & \text{for } x \text{ in the right matrix} \end{cases}$$

Vivian Dornelas, Pablo de Castro, Justin M. Calabrese, William F. Fagan, and Ricardo Martinez-Garcia, 2023

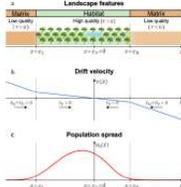
Pablo de Castro

Active Matter & Spatial Ecology

Reaction-Diffusion-Advection Equation

$$\frac{\partial u(x,t)}{\partial t} = r(x)u(x,t) - \gamma u(x,t)^2 + D \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x} (v(x)u(x,t))$$

birth death by competition diffusion advection due to attraction



Heterogeneous net birth rate

$$r = r_H > 0 \quad \text{for } x \text{ in the habitat}$$

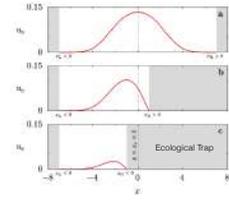
$$r = r_M < 0 \quad \text{for } x \text{ in the matrix}$$

Pablo de Castro

Active Matter & Spatial Ecology

Stationary population spread for absorbing edges

$$r_M \rightarrow -\infty$$



Historical geographical range has been observed in Nature

Pablo de Castro

Active Matter & Spatial Ecology

Critical habitat for absorbing edges

$$r_M \rightarrow -\infty$$

Without attractive location

Critical habitat size

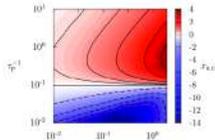
$$L_c = \pi \sqrt{D/r}$$

Verified for bacteria under radiation

Increasing diffusion kills population

With attractive location

Critical edge location



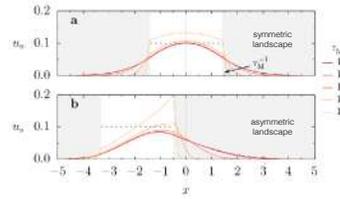
Increasing diffusion saves population
Drift "Paradox"

Pablo de Castro

Active Matter & Spatial Ecology

Fleeing harsh matrix may be worse!

Population spread for finite $r_M < 0$



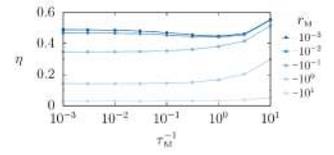
Habitat edge as ecological trap itself

Pablo de Castro

Active Matter & Spatial Ecology

Fleeing harsh matrix may be worse!

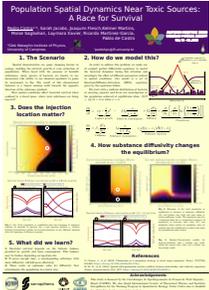
Remaining population fraction for finite $r_M < 0$



Habitat edge as ecological trap itself

Pablo de Castro

Active Matter & Spatial Ecology



Pablo de Castro

Population spread near a toxic source



Pedro Cintra
University of Campinas

Active Matter & Spatial Ecology

Concluding Remarks

Many organisms can be modelled as self-propelled random walkers with interactions

The diffusion equation cannot be used for too-persistent particles even when the diffusively covered area increases linearly in time

The formation of agglomerates is non-monotonic and highly dependent on biological variability

Population spread depends non-trivially on the landscape attractiveness properties

In the presence of a toxic, there are optimal injection points and diffusivities to kill population

A promising area in Physics is the understanding of the movement of life



Pablo de Castro

Active Matter & Spatial Ecology



Pablo de Castro

Soft Matter at IFT & Sirius!



Active Matter & Spatial Ecology



Collaborators



Andressa Vila-Tomealba



Rodrigo Soto



Peter Sollich



Pedro Cintra



Mauricio Rojas-Vega



Vivian Domatas



Ricardo Martinez-Garcia

Pablo de Castro

Active Matter & Spatial Ecology



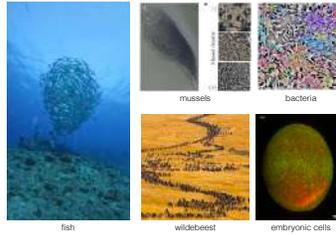
**Collective Dynamics of Moving Organisms:
The Statistical Physics of Self-Propelled Particles**

Pablo de Castro

ICTP South American Institute for Fundamental Research
São Paulo State University



We see patterns in collections of moving organisms **across scales**



Boltzmann



Einstein

Why and how do organisms behave collectively?

Different driving mechanisms

Different environmental conditions

Why some phenomena are common such as

aligned regions ("polar order") or **dense regions** ("phase separation")?

Explanation should be simple

Statistical physics techniques are useful

But thermodynamic equilibrium is never achieved!

Our Physics Approach



spherical cows

Simple models to gain insights and analytical tractability

Analogy: interacting particles subject to deterministic and stochastic forces

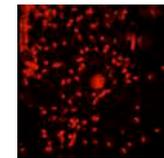
Origin of stochasticity: Ignorance about rapidly-fluctuating forces
We can learn about its statistics



**Collective Dynamics of Moving Organisms:
The Statistical Physics of Self-Propelled Particles**

Pablo de Castro

ICTP South American Institute for Fundamental Research
São Paulo State University



white cells moving to kill invader

Goal

Using simple models and simulations to answer

What are the equations of motion of living organisms?

What is the spatial distribution of living organisms?

How can interactions among organisms and the environment change their distribution?

I. Active Matter

- Free self-propelled particle
- Persistent motion
- Interactions generate clustering
- Consequences

I. Active Matter

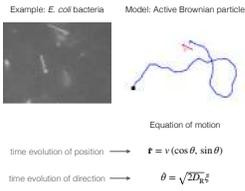
II. Spatial Ecology

II. Spatial Ecology

- How movement bias to attractive regions determines population spatial distributions and critical habitat size

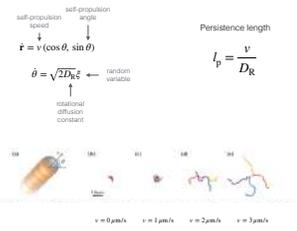
Active Matter

The Free Self-Propelled Particle



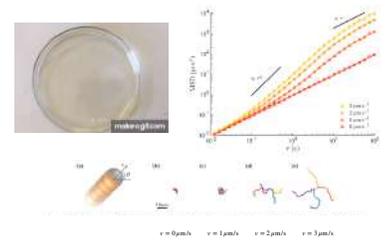
Pablo de Castro Collective Dynamics of Moving Organisms

The Free Self-Propelled Particle



Pablo de Castro Collective Dynamics of Moving Organisms

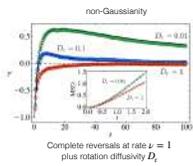
Area covered by **active** diffusive motion grows superlinearly



Pablo de Castro Active Mixtures

True diffusion may take even longer!

Andrés Vila-Torrealba, Cristóbal Chávez-Raboy, Pablo de Castro, and Rodrigo Soto
Physical Review E, 2020

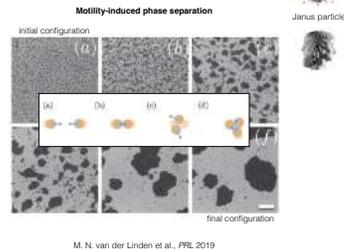


$\text{MSD} \sim t$ is not enough!

Diffusion equation cannot be used!

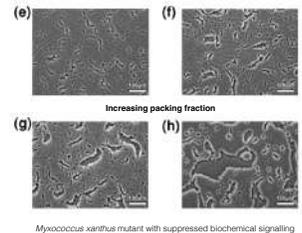
Pablo de Castro Active Mixtures

Interactions: Short-range repulsion



Pablo de Castro Collective Dynamics of Moving Organisms

Clustering in bacterial colonies



Pablo de Castro Collective Dynamics of Moving Organisms

Active Wetting: formation of accumulation layer by active matter on boundaries

Motivation: biofilm initiation & contamination

Model: active Brownian particles + short-range repulsion between particles and with wall

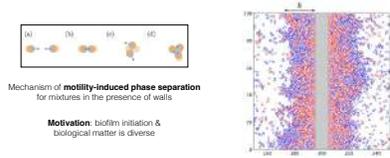
Mechanism of motility-induced phase separation in the presence of walls



Mauricio Rojas-Vega, Pablo de Castro & Rodrigo Soto
Physical Review E, 2023

Pablo de Castro Collective Dynamics of Moving Organisms

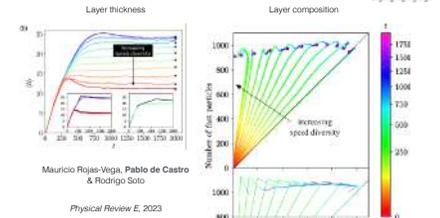
Wetting by Active Mixtures



Mauricio Rojas-Vega, Pablo de Castro & Rodrigo Soto
Physical Review E, 2023

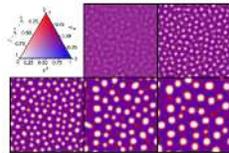
Pablo de Castro Collective Dynamics of Moving Organisms

Surface accumulation by active mixtures is **non-monotonic in time** because particles with certain orientations and speeds get more trapped



Pablo de Castro Collective Dynamics of Moving Organisms

Passive phase separation of mixtures is **also two-stage** due to crowding but evolves via **attractive** mechanism



Phase separation of **protein soup**. Time flows from left to right, top to bottom.

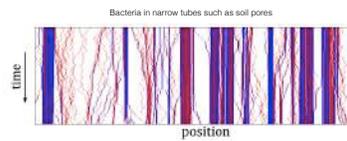
Pablo de Castro & Peter Sollich

Soft Matter 2019
Physical Chemistry Chemical Physics 2017

Pablo de Castro

Collective Dynamics of Moving Organisms

Confinement and population heterogeneity in motility properties changes cluster size distribution



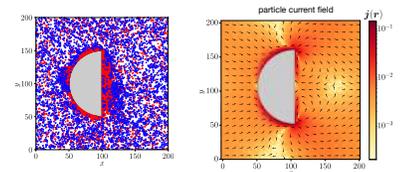
Pablo de Castro, FM Rocha, S Diles, R Soto, P Sollich

Soft Matter 17 (8), 2050-2061, 2021
Soft Matter 17, 9926-9936, 2021

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Collective Dynamics of Moving Organisms

For active mixtures interacting with **asymmetric** obstacles, **rectification** arises in addition to accumulation



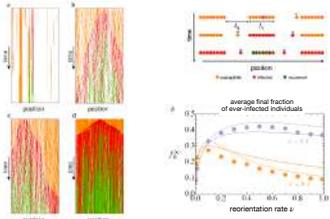
Used to concentrate sperm and bacteria

Mauricio Rojas-Vega, Pablo de Castro & Rodrigo Soto
The European Physical Journal E, 2023

Pablo de Castro

Collective Dynamics of Moving Organisms

Disease spread between **clusters of active particles**
Intermediate reorientation rate maximizes infections

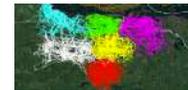


Pablo de Castro, Felipe Urbina, Ariel Norambuena & Francisca Guzmán-Lastra
Physical Review E, 2023

Pablo de Castro

Collective Dynamics of Moving Organisms

Large spatial and temporal scales



Wolves GPS tracking data



Reproduction and competition are important

Large spatial scales \implies Accumulation by persistence + contact reaction is **absent**

Long time scales \implies **Non-persistent diffusion** models can be used

Environmental conditions and **ecological** processes are relevant

Pablo de Castro

Collective Dynamics of Moving Organisms

Spatial Ecology

Fisher-Kolmogorov Equation

Reaction-Diffusion Equation

$u(x, t)$ \equiv density of individuals at x and t

$$\frac{\partial u}{\partial t} = ru - \gamma u^2 + D \frac{\partial^2 u}{\partial x^2}$$

temporal change net birth death by competition movement by diffusion

In regions with high densities, there is net death due to competition

Stationary solution for unbounded systems & small perturbation as initial condition: $u(x) = r/\gamma$

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Collective Dynamics of Moving Organisms

Attractive location generates movement bias



$$\dot{x} = -\frac{x - x_p}{\tau_p} + \sqrt{2D}\xi$$

Overdamped Brownian particle confined by a harmonic potential

[Fits data for hundreds of species](#)

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Collective Dynamics of Moving Organisms

Fisher-Kolmogorov-Ornstein-Uhlenbeck Equation

Reaction-Diffusion-Advection Equation

$u(x, t)$ \equiv density of individuals at x and t

$$\frac{\partial u}{\partial t} = ru - \gamma u^2 + D \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x}(vu)$$

temporal change net birth death by competition movement by diffusion advection due to attraction

$$v(x) = -\frac{x - x_p}{\tau_p}$$

Stationary solution for unbounded systems & small perturbation as initial condition: **Gaussian** around x_p

Pablo de Castro

Collective Dynamics of Moving Organisms



IFT - UNESP
INSTITUTO DE FÍSICA TEÓRICA



FAPESP Scientific Report 2023
Fluctuations and Non-Hermiticity in Nematic Materials

Project: 2023/05765-7

Beneficiary: Rui Aquino dos Santos da Silva
Supervisor: Nathan Jacob Berkovits

Time period of the entire project: 01/11/2023 – 01/11/2025
Time period in which this report refers to: 01/11/2023 – 08/12/2023

Summary of the Project

In recent years, the physics of Condensed Matter has substantially widened its horizons far beyond its traditional boundaries. Macroscopic quantum phenomena as superconductivity [1], the quantum Hall effect [2] and Bose-Einstein condensation [3] have been observed in new exciting materials, and, in some of those, have been applied in the development of new technologies.

From a theoretical point of view, the “Quantum Field Theory (QFT)”, initially formulated for approaching problems in high-energy physics, stands out in its applications in Condensed Matter and Statistical Mechanics [4 - 6], especially in strongly correlated systems. Important examples are the so-called “superconducting cuprates” [7], heavy fermion systems such as “ruthenates” [8], and the “iron-based superconductors” [9], among others.

The application of QFT techniques in Condensed Matter systems provides relevant information about thermodynamic and transport properties both in equilibrium and out of thermodynamic equilibrium. Generally, QFT is used to build up models that exploit the physics of low energy and large correlation lengths. These became specially important in the regime near a phase transition, classic or quantum, where usual perturbative techniques cannot be applied.

In this project, we will be interested not only in the critical regime of these systems, but specially on its dynamical properties. Focussing on metallic phases, its electronic properties are described by electron fluids, which are special cases of quantum liquids. Similar to its classical analogs, they display a plethora of phase transitions to anisotropic, non-homogenous gapless phases, generally known as quantum liquid crystals. The Landau Theory of Fermi Liquids has provided the paradigms to describe electronic quantum liquids since the late 1950's [10, 11]. Usually, in order to characterize a given phase of a system, one needs to understand its symmetries. These symmetries state the form and properties of the static part of a given functional, for example, the Hamiltonian or the static free energy. Although this is enough to define a huge number of properties of matter, to fully characterize its dynamical quantities, more information is needed.

Different approaches are used to time evolve a many-body system. One can use microscopic arguments, for example, considering the Schrödinger dynamics of a single fermion, to compute the effective time evolution of a large number of fermionic fields. Also, one can give phenomenological arguments to infer the properties of the critical evolution of systems near criticality [12], or the evolution of particle-number fluctuations to describe the propagating modes within electron liquids [13]. For systems with different symmetries, one can think of its evolution in time through order-parameter fluctuations.

In particular, order-parameter fluctuations of Fermi liquids are a rich research field from the theoretical and experimental point of view. Although the seminal zero sound excitation, a sound mode propagating in a three-dimensional fermion liquid, was computed by Landau and measured in experiments with He3 at low temperatures in the 50 and 60's [14, 15], this field regained relevance with the increasing interest in low-dimensional systems. In this project, we will focus on the study of the dynamical nematic fluctuations of the normal phase of real materials, such as iron-based superconductors or

cuprates. Using quantum field theoretical approaches, we will compute the dynamical response of the Ising-nematic order parameter. The effect of collective mode excitations will be studied in detail, in which non-hermitian phenomena was recently proposed [16 – 18] to appear.

The importance of non-hermitian (NH) phenomena can be realized by noting that non-hermitian Hamiltonians are widely used in effective descriptions of a variety of phenomena. Photonic systems [19 – 23], semimetals, insulators [24 – 27], and interacting systems [28 – 33] are some examples in which NH phenomena emerge. One prominent feature of NH Hamiltonians is the appearance of exceptional points (EPs) in their spectra [34 – 36], which arise for specific values of the parameter space. Exceptional points are spectral degeneracies where the eigenvectors coalesce and the NH Hamiltonian becomes defective, inducing remarkable topological properties [37,38] that have been observed and explored in different experimental setups.

Finally, this project aims to phenomenologically study an interesting non-hermitian degeneracy that emerges in the collective modes spectrum of a class of Fermi liquids with multipolar interactions. In particular, the quadrupolar interaction induces an isotropic-nematic phase transition in the strong attractive channel. Due to the fact that the non-hermitian degeneracy, called exceptional point, appears for weak attractive interaction [16 - 18], we propose to model and study the dynamics of real compounds which present nematic fluctuations, such for instance iron-based superconductors. This understanding could help us to have a deeper insight into the intricate phase diagram of these materials. We expect to compare our results with experimental data recently obtained.

Realizations of the period

We start our work on the ICTP-SAIFR on the IFT-UNESP on November, 1th. We focussed in working on three major collaborations. In the following we will expose each one of the collaborations, together with a small text motivating each project.

First of all, we are working together with Dr. Rafael Fernandes, from University of Minnesota (USA), and Dr. Joerg Schmalian from Karlsruhe Institute of Technology (Germany). The project has the goal to understand the impact of nematic fluctuations on the Hall viscosity of electronic fluids. In the follow, we present a small text on the project.

“Electronic nematic order and fluctuations are of great importance to a wide class of correlated electronic materials, such as unconventional superconductors, doped topological insulators, and twisted moiré systems. Because of the intertwining between nematicity and elasticity, the manifestations of nematic fluctuations on elastic properties of the lattice, such as the shear modulus, have been widely investigated. In this project, we explore the impact of nematic fluctuations on the elastic properties of the electronic fluid itself. In particular, we focus on the Hall viscosity coefficient, which is the electronic counterpart of the dissipationless generation of stress by a time-varying strain in the presence of time-reversal symmetry-breaking. We consider the case of graphene, which is a model electronic fluid, and compute the contribution to the Hall viscosity arising from electronic nematicity, highlighting the role played by dynamic nematic fluctuations.”

Also, we are working on a project with the theoretical condensed matter group at the University of State of Rio de Janeiro (UERJ), with Dr. Daniel G. Barci (UERJ) and Nathan O. Silvano from UERJ

and Center for Advanced Systems Understanding (Germany). The goal of the project is to theoretically study the topological response of the exceptional point in nematic materials, using light pulses, the same experimental technique that made Pierre Agostini, Ferenc Krausz and Anne L’Huillier being granted with the Nobel prize in 2023. Regarding this project, here follows

“Non-hermitian degeneracies, the so called exceptional points, are singularities which appears in the collective mode spectrum of Fermi liquids with high angular momentum interactions. In this project we want to know if the topology of the exceptional points can be probed using electromagnetic response of Fermi Liquids. From the experimental perspective, the study of collective modes of strongly correlated systems is quite involved. Here we will theoretically work with a specific type of measurement, time-resolved spectroscopy. These exciting time domain measurements allow us to use light as a external parameter and explore order parameter fluctuations. In particular, the structure of the collective modes and in particular of the exceptional points was already theoretically computed in pump-probe setups before [17]. Now, however, we want to propose an set up to probe the topology of the exceptional point using these type of experiments.”

Finally, we are working with Pedro Ventura Paraguassú, from PUC – RJ, on a parallel work on stochastic thermodynamics, continuing a project that we have been working in the last two years.

“When dealing with Brownian systems, fluctuations in energy and energy transfer arise due to the inherent statistical behavior of Brownian motion. These fluctuations are interpreted and studied within the framework of Stochastic Thermodynamics. In this study, we investigate heat in overdamped Brownian systems driven by a simple protocol designed to introduce a bias in the particle's motion. Earlier predictions for such systems proposed that heat would be equal to work, implying a Gaussian random variable due to the absence of potential energy. However, the necessity of incorporating kinetic energy into the heat formula for overdamped systems, a result recently demonstrated, demands new investigation. This reveals that heat no longer adheres to Gaussian behavior due to the inclusion of kinetic energy. We delve into the non-Gaussian fluctuations of heat by systematically studying the accurate heat formula, computing essential central moments, probability density, and comparing these results with the incorrect Gaussian scenario using the Kullback-Leibler distance.”

Plans for next period

We will obtain objective and measurable results of two kinds: high impact factor publications and human resources formation.

● Publications

We expect to publish at least four article related to this project in high quality journals during the next year. We will expose each one of our current work in preparation as follows:

- Rui Aquino, Rafael M. Fernandes, Joerg Schmalian. Impact of nematic fluctuations on the Hall viscosity of electronic fluids. *Work in progress*.
- Nathan O. Silvano, Rui Aquino, Daniel G. Barci. Laser control of XY-nematic fluctuations I: Pomeranchuk instability. *Work in progress*.

- Rui Aquino, Nathan O. Silvano, Daniel G. Barci. Laser control of XY-nematic fluctuations II: exceptional points and its topology. *Work in progress*.
- Pedro V. Paraguassú, Rui Aquino. Non-Gaussian heat fluctuations for driven Brownian systems. *Work in progress*.

- Congresses

The project advances are expected to be communicated in national as well as international congresses and workshops. The international congresses and seminars will be organized by American Physical Society and by the research groups in Minnesota. In fact, we intend to communicate our work in the March Meeting, which will be held in Minnesota this year.

Moreover, we intend to start new collaborations with Brazilian and German groups, specially in Leipzig and Campinas.

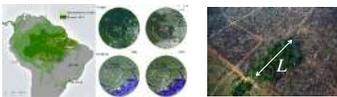
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Heterogeneous landscapes

Fragmented habitat due to **deforestation**-like processes



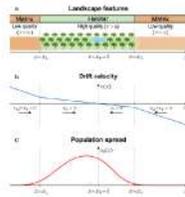
Critical Habitat Size

Pablo de Castro

Collective Dynamics of Moving Organisms

Heterogeneous landscapes

Effect on population spatial distribution



Heterogeneous net birth rate

$$r = r_H > 0 \quad \text{for } x \text{ in the habitat}$$

$$r = r_M < 0 \quad \text{for } x \text{ in the matrix}$$

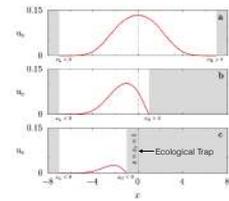
Vivian Dornelas, Pablo de Castro, Justin M. Calabrese, William F. Fagan, and Ricardo Martinez-Garcia

Submitted (2023)

Pablo de Castro

Collective Dynamics of Moving Organisms

Stationary population density distribution for instantaneous death in the matrix



Historical geographical range has been observed in Nature
 If **attractive** location is in the **matrix**, it becomes ecological trap
 Even so, population may survive!
 There is **window of opportunity** for conservation biology

Pablo de Castro

Collective Dynamics of Moving Organisms

Critical habitat for instantaneous death in the matrix

Without attractive location

Critical habitat size

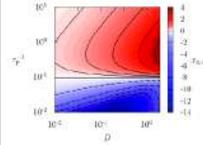
$$L_c = \pi \sqrt{D/r} \quad \text{net birth rate}$$

Verified for bacteria under radiation

More diffusive individuals require more habitat to avoid extinction

With attractive location

Critical edge location



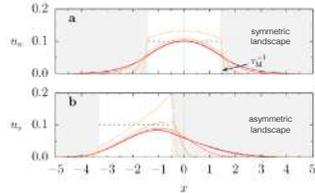
More diffusive individuals may require less habitat to avoid extinction: **Drift "Paradox"**

Pablo de Castro

Collective Dynamics of Moving Organisms

Fleeing harsh matrix may be worse!

Population spread for **non-instantaneous death** in the matrix



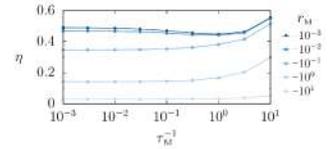
Habitat edge as ecological trap itself

Pablo de Castro

Collective Dynamics of Moving Organisms

Fleeing harsh matrix may be worse!

Remaining population fraction for non-instantaneous death in the matrix



Habitat edge as ecological trap itself

Pablo de Castro

Collective Dynamics of Moving Organisms

Concluding Remarks

Essential features of organisms motion can be incorporated into simplified models of self-propelled random walkers with interactions to obtain insights

Normal diffusion models cannot always be used to model active particles

Persistent motion generates accumulation and, as a result, several behaviors in active matter models:

- confinement and population heterogeneity in motility can change cluster sizes dramatically
- non-monotonic time-dependence of surface accumulation properties for mixtures
- spontaneous current emergence for mixtures in the presence of asymmetric obstacles
- disease or information spread is optimal for intermediate persistence

For larger scales, ecology matters while persistent motion features may matter less

Spatial distributions depend non-trivially on properties of landscape attractiveness

Models predict that deforestation patterns change critical habitat sizes and may affect policies



Pablo de Castro

Collective Dynamics of Moving Organisms



School and Workshop on Active Matter at ICTP-SAIFR

São Paulo, Brazil

30 September to 4 October, 2024

Rodrigo Soto, Santiago
Kinetic Models of Active Suspensions

Peter Sollich, Göttingen
Phase behavior and glassy dynamics

Julia Yeomans, Oxford
Active nematics and tissues

Pablo de Castro

Collective Dynamics of Moving Organisms



Collaborators



Pablo de Castro

Collective Dynamics of Moving Organisms

Active mixtures interacting with walls and obstacles



Mauricio Rojas-Vega¹, Pablo de Castro^{2,*} & Rodrigo Soto³

¹ Institute of Science and Technology Austria, Austria

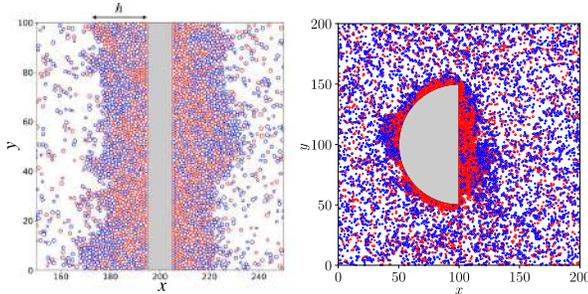
² ICTP-SAIFR & Universidade Estadual Paulista, Brazil

³Departamento de Física, FCFM, Universidad de Chile, Chile



Introduction

- Microorganisms interact with obstacles inside the host body where they live
- Active matter tends to accumulate on hard surfaces due to persistent motion



- For asymmetric obstacles, particle rectification currents arise besides accumulation/wetting
- Biological active matter is diverse. Individuals have distinct self-propulsion speeds
- **Which behaviors emerge from interactions of active mixtures with large obstacles?**

Model

- Consider repulsive active Brownian particles in two dimensions
- Half are **fast**, self-propulsion $v_f = v_0(1 + \delta)$
- Half are **slow**, self-propulsion $v_s = v_0(1 - \delta)$
- Here δ is the self-propulsion speed “diversity”

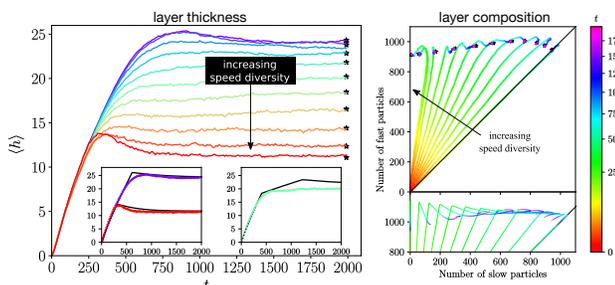
Flat wall [1]

Transient evolution: Layer thickness

- The thickness shows an overshoot before reaching the stationary state

Transient evolution: Layer composition

- The layer composition evolves in two stages

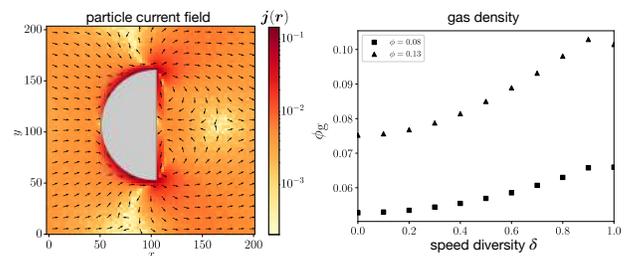


Kinetic theory

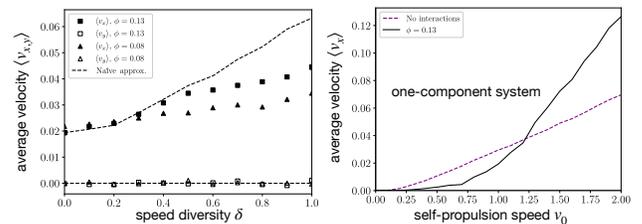
- Absorption-evaporation balance *per type* sets number of particles in the layer
- Absorption rate is proportional to self-propulsion speed and the gas density
- Evaporation rate depends on composition of the layer & reorientation rate at interface
- Average escape number (avalanches) increases after internal reorientation

Asymmetric obstacles [2]

- Lever rule is violated: additional density is not absorbed by the wetting layer



- Rectification is amplified by speed diversity
- Why? The rectification velocity increases superlinearly with the self-propulsion speed



References

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Acknowledgments

M.R.-V. and R.S. were supported by Fondecyt No. 1220536 & Millennium Science Initiative ANID No. NCN19_170D, Chile, and P.d.C. by FAPESP Nos. 2021/10139-2, 2022/13872-5, 2021/14335-0, Brazil.

Contact

pablo.castro@unesp.br
pablodecastro.weebly.com



7 List of Submitted (not published) Works in the Report Period

This work has been submitted but not yet published.

- **Authors:** Vivian Dornelas, Pablo de Castro, Justin M. Calabrese, William F. Fagan, Ricardo Martinez-Garcia
Title: “How movement bias to attractive regions determines population spread and critical habitat size”
Status: Submitted to *Journal of Theoretical Biology*.

1 How movement bias to attractive regions determines spatial
2 population distribution and critical habitat size

3 Vivian Dornelas^{*1,2}, Pablo de Castro^{*1}, Justin M. Calabrese^{3,4,5}, William F. Fagan⁵,
4 and Ricardo Martinez-Garcia^{†3,1}

5 ¹ICTP – South American Institute for Fundamental Research and Instituto de Física Teórica,
6 Universidade Estadual Paulista – UNESP, São Paulo, Brazil.

7 ² National Institute of Chemical Physics and Biophysics - Akadeemia Tee 23, Tallinn 12618, Estonia.

8 ³Center for Advanced Systems Understanding (CASUS); Helmholtz-Zentrum Dresden-Rossendorf
9 (HZDR), Görlitz, Germany.

10 ⁴Department of Ecological Modelling, Helmholtz Centre for Environmental Research – UFZ, Leipzig,
11 Germany.

12 ⁵Department of Biology, University of Maryland, College Park, MD, USA.

13 **Abstract**

14 Ecologists have long investigated how the demographic and movement parameters
15 of a population determine its spatial spread and the critical habitat size that can sus-
16 tain it. Yet, most existing models make oversimplifying assumptions about individual
17 movement behavior, neglecting how landscape heterogeneity influences dispersal. We
18 relax this assumption and introduce a reaction-advection-diffusion model that describes
19 the spatial density distribution of a population with space-dependent movement bias
20 toward preferred regions, including avoidance of degraded habitats. In this scenario, the
21 critical habitat size depends on the spatial location of the habitat edges with respect
22 to the preferred regions and on the intensity of the movement bias components. In
23 particular, we identify parameter regions where the critical habitat size decreases when
24 diffusion increases, a phenomenon known as the “drift paradox”. We also find that
25 biased movement toward low-quality or highly populated regions can reduce the pop-
26 ulation size, therefore creating ecological traps. Our results emphasize the importance
27 of species-specific movement behavior and habitat selection as drivers of population
28 dynamics in fragmented landscapes and, therefore, the need to account for them in the
29 design of protected areas.

*These authors contributed equally to this work and share first authorship

†Correspondence: r.martinez-garcia@hzdr.de

30 1 Introduction

31 Habitat destruction and fragmentation result in smaller and more isolated suitable habitat
32 patches where extinctions are more likely to occur (Franklin et al., 2002; Lord and Norton,
33 1990; Nauta et al., 2022). The viability of a population in each of these patches depends
34 on the balance between growth inside the patch and population losses, mainly stemming
35 from dispersal through habitat edges. The interplay between these two processes sets the
36 minimum area required to sustain the population and defines a patch-size threshold (Kier-
37 stead and Slobodkin, 1953). Thus, understanding the interaction between demographic and
38 dispersal processes is key to determining critical patch sizes across species, which has im-
39 portant implications for conservation, such as in the design of protected areas or ecological
40 corridors (Cantrell and Cosner, 1999; Ibagon et al., 2022). Additionally, determining the
41 expected spatial pattern of population density in patches larger than the critical size can
42 improve understanding of population responses to further habitat destruction.

43 The importance of critical patch sizes and population spread in finite habitat patches
44 has led researchers to test model predictions in microcosm experiments using microbial pop-
45 ulations (Lin et al., 2004; Perry, 2005) as well as in large-scale experiments and observations
46 (Ferraz et al., 2003; Pereira and Daily, 2006; Turner, 1996). Despite the biological under-
47 standing gained from these and other empirical studies, key aspects of complexity remain
48 absent from theoretical modeling of critical patch size phenomena. The most common mod-
49 els to determine critical habitat sizes consist of a reaction-diffusion equation describing the
50 spatio-temporal dynamics of a population density in a bounded region. Within this family of
51 models, the simplest ones assume purely diffusive dispersal coupled with exponential growth
52 and are commonly called KISS models (Kierstead and Slobodkin, 1953; Skellam, 1951). Due
53 to these highly simplified assumptions, KISS models lead to analytical expressions for the
54 critical patch size.

55 More recently, researchers have refined movement descriptions by including space-dependent
56 diffusion within the patch (Colombo and Anteneodo, 2018; Dos Santos et al., 2020), re-
57 sponses to habitat edges (Cronin et al., 2019; Fagan et al., 1999; Maciel and Lutscher, 2013),
58 and various sources of non-random movement, such as a constant external flow (Pachepsy
59 et al., 2005; Ryabov and Blasius, 2008; Speirs and Gurney, 2001; Vergni et al., 2012) or a
60 chemoattractant secreted by the population (Kenkre and Kumar, 2008). Other studies have
61 explored more complex growth dynamics, such as Allee effects (Alharbi and Petrovskii, 2016;
62 Cronin et al., 2020), time-varying environments (Zhou and Fagan, 2017), or heterogeneity in
63 population growth, either through time-dependent demographic rates (Ballard et al., 2004;
64 Colombo and Anteneodo, 2016) or by introducing a finer spatial structure of habitat quality
65 within the patch (Cantrell and Cosner, 2001; Fagan et al., 2009; Maciel and Lutscher, 2013).
66 Finally, a few studies have combined space-dependent demographic rates with migration to-
67 ward higher quality regions within the patch, in the presence of an environmental gradient,
68 to determine critical patch sizes (Cantrell and Cosner, 1991, 2001; Cantrell et al., 2006) or
69 population spatial distributions depending on the type of boundary conditions (Belgacem

70 and Cosner, 1995).

71 Despite this significant endeavor to refine classical KISS models, some movement fea-
72 tures which are present in most species and which directly impact population spread remain
73 underexplored. For example, individuals often show a tendency to move toward certain habi-
74 tat regions where they concentrate, which makes population ranges smaller than the total
75 amount of habitat available (Kapfer et al., 2010; Van Moorter et al., 2016). While a con-
76 siderable effort has focused on understanding how and why individuals show these patterns
77 of space use (Jeltsch et al., 2013; Nathan et al., 2008), their population-level consequences,
78 especially in fragmented landscapes, have been less explored. Motivated by colonial central-
79 place foragers such as ants, beavers, and colonial seabirds, one particular study obtained,
80 numerically, the critical patch size when the home-range centers for all the individuals in the
81 population are at the center of the habitat patch (Fagan et al., 2007). Overall, however, the
82 lack of a more general theoretical framework limits the current understanding of how habi-
83 tat selection within a fragmented landscape determines the spatial distribution and critical
84 patch size for a given population.

85 Here we take a new step to fill this theoretical gap by extending classical KISS models to
86 account for space-dependent deterministic movement. We study how this additional move-
87 ment component influences population spread in a heterogeneous one-dimensional landscape
88 and the critical habitat patch size that ensures population survival. We consider the simple
89 one-dimensional scenario with a finite high-quality habitat patch embedded in a low-quality
90 “matrix” with high mortality. Using both numerical and analytical methods, we measure
91 critical patch size and spatial patterns of population density for different matrix mortality
92 levels. We also vary the intensity of two deterministic space-dependent movement compo-
93 nents relative to random dispersal: a bias to preferred landscape locations and avoidance
94 of degraded habitats. We find that the total population lost due to habitat degradation
95 and the critical patch size depend nonlinearly on the parameters that control the differ-
96 ent movement components as well as on the spatial distribution of habitat relative to the
97 landscape regions where individuals move more slowly. Overall, our results emphasize the
98 importance of incorporating covariates between movement behavior and landscape features
99 when investigating population dynamics in heterogeneous landscapes.

100 2 Material and Methods

101 2.1 Model formulation

102 We consider a one-dimensional heterogeneous landscape with a habitat patch embedded in
103 an infinite matrix (see Fig. 1a). The left and right habitat patch edges are located at $x = x_L$
104 and $x = x_R$, respectively, and the habitat patch size is $L = |x_R - x_L|$. The landscape is
105 occupied by a single-species population, which we describe via a continuous density field
106 $u(x, t)$. This population density changes in space and time due to demographic processes
107 and dispersal. For the birth/death dynamics, we assume that the population follows logistic
108 growth with net reproduction rate r and intraspecific competition intensity γ . The net

109 growth rate is constant within each type of region but different between regions: $r(x) =$
 110 $r_H > 0$ inside the habitat patch (high-quality, low-mortality region) and $r(x) = r_M < 0$
 111 in the matrix (low-quality, high-mortality region). The matrix mortality rate r_M defines
 112 the degree of habitat degradation, with the limit $r_M \rightarrow -\infty$ representing complete habitat
 113 destruction. For finite mortality rates, whether an individual dies in the matrix or not is
 114 determined by the mortality rate itself and the time the individual spends in the matrix.
 115 Therefore, when the matrix is not immediately lethal, the population density outside the
 116 habitat patch is not zero. For dispersal, we consider two different movement components:
 117 random dispersal with constant diffusion coefficient D , and a deterministic tendency of
 118 individuals to move toward attractive regions with space-dependent velocity $v(x)$, therefore
 119 accounting for the effect of landscape heterogeneity in movement behavior. Importantly,
 120 this attractive term in our model generates movement bias toward regions that are not
 121 necessarily of higher habitat quality. The actual velocity of an individual is thus equal to
 122 $v(x)$ plus a stochastic contribution that comes from diffusion. Combining these demographic
 123 and movement processes, the dynamics of the population density is given by

$$124 \quad \frac{\partial u(x, t)}{\partial t} = r(x)u(x, t) - \gamma u(x, t)^2 + D \frac{\partial^2 u(x, t)}{\partial x^2} - \frac{\partial}{\partial x} \left(v(x)u(x, t) \right). \quad (1)$$

125 The functional form of the advection velocity $v(x)$ depends on landscape features, with
 126 attractive locations corresponding to x coordinates with slower velocity. We consider two
 127 different types of attractive regions.

128 First, we incorporate a tendency to move toward an attractive *location* with velocity
 129 $v_P(x)$. This term could represent, for example, attraction toward a chemoattractant source
 130 or toward a special resource, such as a watering hole. We choose

$$131 \quad v_P(x) = -\tau_P^{-1}(x - x_P), \quad (2)$$

132 where we assumed that the velocity at which individuals tend to move toward attractive
 133 landscape regions increases linearly with the distance to the focus of attraction. This is
 134 similar to how simple data-driven models for range-resident movement implement attraction
 135 to home-range center at the individual level (Dunn and Gipson, 1977; Noonan et al., 2019).
 136 The prefactor τ_P^{-1} is the attraction rate toward the attractive location and defines the
 137 typical time that individuals take to re-visit x_P . In the following, we use $x_P = 0$ in all our
 138 calculations, such that the locations of the habitat edges are measured relative to the focus
 139 of attraction.

140 Second, we consider that individuals in the matrix tend to return to the habitat patch
 141 with velocity $v_M(x)$, and therefore, we incorporate an additional attraction term biasing
 142 movement from the matrix toward its closest habitat edge. Again, we consider a linear

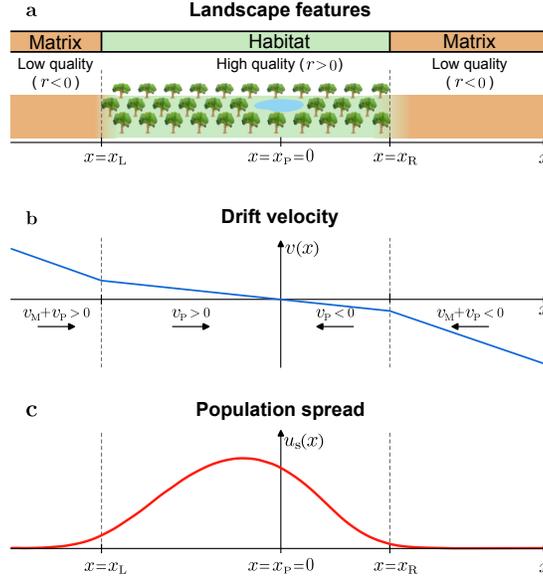


Figure 1: Model schematics. (a) Landscape features, showing a high-quality habitat ($r > 0$) and an attractive location (represented as a watering hole at position $x = x_p = 0$) surrounded by low-quality matrix regions ($r < 0$). Habitat edges are located at $x = x_L$ and $x = x_R$. In this example, x_R is positive. The total habitat size is $L = |x_R - x_L|$. (b) Spatial dependence of the drift velocity (deterministic movement component). Velocity v_p points to the attractive location [Eq. 2]. For individuals in the matrix, an additional term (v_M) points to the edges [Eq. 3]. (c) Emerging stationary population density distribution $u_s(x)$, peaking to the left of $x = 0$.

143 spatial dependence, but now only for individuals in the matrix:

$$144 \quad v_M(x) = \begin{cases} -\tau_M^{-1}(x - x_L), & x < x_L \\ 0, & x_L \leq x \leq x_R \\ -\tau_M^{-1}(x - x_R), & x > x_R \end{cases} \quad (3)$$

145 The prefactor τ_M^{-1} is the edge attraction rate that modulates the strength of the matrix-to-
 146 habitat attraction $v_M(x)$. In the habitat, $v_M(x) = 0$, whereas in the matrix, it is equal to τ_M^{-1}
 147 multiplied by the distance to the closest edge. Moreover, the velocity $v_M(x)$ always points
 148 toward the habitat patch, therefore biasing the movement of the individuals in the matrix
 149 toward the habitat-matrix edges. This matrix avoidance drift assumes that individuals
 150 remain aware of the direction in which the favorable habitat is located, which extends
 151 previous models for movement response to habitat edges that act only at the habitat-matrix
 152 boundary (Cronin et al., 2019; Fagan et al., 1999; Maciel and Lutscher, 2013).

153 Putting together the movement toward the attractive location and the matrix avoidance
 154 bias, we obtain a velocity of the form $v(x) = v_p(x) + v_M(x)$ (see Fig. 1b for $v(x)$ and Fig. 1c
 155 for the population spread emerging from it). We highlight that, for an infinite habitat
 156 patch, the total population is not infinite since attraction concentrates individuals around
 157 the attractive location, leading to a limited total population through competition. As a
 158 result, the population goes to zero at some finite distance from the attractive location and
 159 therefore the maximum drift velocity $v(x)$ that emerges in the system is finite. We provide

a summary of the model parameters in Table 1.

Sym.	Parameter	Dimensions
r_H	Habitat net growth rate	time ⁻¹
r_M	Matrix net rate	time ⁻¹
γ	Intensity of intraspecific compet.	(time \times density) ⁻¹
D	Diffusion coefficient	space ² /time
x_P	Center attractive location	space
x_L	Position of left habitat edge	space
x_R	Position of right habitat edge	space
τ_P^{-1}	Attraction rate to attractive location	time ⁻¹
τ_M^{-1}	Matrix-to-habitat attraction rate	time ⁻¹

Table 1: Summary of model parameters with symbols and dimensions. Units are arbitrary. Specific values are provided in figure captions.

160

161 2.2 Model analysis

162 We analyze the stationary solutions of Eq. (1) using a combination of a semi-analytical
 163 method and numerical simulations of the full nonlinear equation. We use both approaches
 164 in the $r_M \rightarrow -\infty$ limit and perform only numerical simulations in the more general case
 165 with finite r_M .

166 2.2.1 Semi-analytical determination of critical habitat for $r_M \rightarrow -\infty$

167 In the $r_M \rightarrow -\infty$ limit, individuals die instantaneously upon reaching the matrix, and we
 168 can replace the dynamics of the population density in the matrix by absorbing boundary
 169 conditions at the habitat edges, $u(x_L, t) = u(x_R, t) = 0$. In this regime, the movement
 170 component that attracts individuals to the habitat edge, v_M , has no effect on the dynamics.
 171 In order to determine the critical habitat configurations (x_L, x_R) that lead to population
 172 extinction for a given set of movement parameters, we analyze the steady state of the
 173 linearized version of Eq. (1) and ask when the extinction solution $u(x, t \rightarrow \infty) \equiv u_s(x) = 0$
 174 is the only possible solution. Such linearization is possible because the transition occurs from
 175 a small population to no population. This approach has been successfully used elsewhere
 176 (Okubo, 1972). To perform this analysis, we neglect the quadratic term in the logistic growth
 177 and take the limit $t \rightarrow \infty$ in Eq. 1, which is equivalent to setting $\partial_t u(x, t) = 0$. In this limit,
 178 Eq. 1 becomes an ordinary differential equation whose solution can be easily obtained from
 179 a symbolic calculation software. The solution reads

$$180 \quad u_s(x) = \exp\left(-\frac{x^2}{2\tau_P D}\right) \left[a H_{r\tau_P} \left(\frac{x}{\sqrt{2D\tau_P}} \right) + b {}_1F_1 \left(-\frac{r\tau_P}{2}; \frac{1}{2}; \frac{x^2}{2D\tau_P} \right) \right], \quad (4)$$

181 where a and b are constants that depend on the boundary conditions. ${}_1F_1$ is the confluent
 182 hypergeometric function of the first kind, and $H_n(x)$ is the Hermite polynomial, with n
 183 being a real, not necessarily integer, number (Arfken and Weber, 1999).

184 Imposing absorbing boundary conditions at the habitat edges on Eq. 4, we obtain a
 185 system of two equations for a and b that can be used to determine whether the solution
 186 $u_s(x) = 0$ is the only one possible. For this system of equations to have non-trivial solutions

187 (that is, different from $a = b = 0$), its determinant has to be zero. With this condition for
 188 the determinant and assuming that x_L is fixed, we obtain a transcendental equation in x_R
 189 that we can solve numerically to obtain the critical location of the right habitat edge, $x_{R,C}$.
 190 The numerical solution to this transcendental equation is obtained in the following way.
 191 First, we take the case whose solution we know analytically ($\tau_P^{-1} = 0$). Then, we increase
 192 τ_P^{-1} by small increments and use as initial guess the solution to the previous τ_P^{-1} considered.

193 **2.2.2 Numerical solution of the nonlinear model equation**

194 We perform all numerical simulations using a standard Euler scheme that is central in space
 195 and forward in time (Press, 2007). The initial condition for the density, $u(x, 0)$, consists of
 196 a small random spatial fluctuation that is uniformly distributed between 0 to 10^{-4} , except
 197 the completely destroyed habitat (the region with $r_M \rightarrow -\infty$), where the density is set to
 198 zero. To simulate an infinite region, we take a simulation box (with absorbing boundary
 199 conditions) large enough so that in the steady state the population goes to zero (or at
 200 least less than 10^{-20}) within it. We remind that for infinite systems, the total population
 201 is not infinite due to attraction. For a completely destroyed habitat, absorbing boundary
 202 conditions were applied at the edges of the habitat. In order to calculate $x_{R,C}$, we integrate
 203 Eq. 1 for a variety of habitat patch sizes, keeping x_L constant and far enough from the center.
 204 Then, we systematically vary x_R until the population undergoes a critical transition from
 205 survival to extinction (see Fig. 2 for spatial patterns of population density as x_R decreases,
 206 with $x_R > x_{R,C}$).

207 Finally, we also use these numerical solutions of Eq. 1 to measure population loss due to
 208 habitat degradation. For this purpose, we introduce a dimensionless quantity, η , defined as
 209 the total population size sustained by a finite habitat patch of size L divided by the total
 210 population size sustained by an infinite habitat patch. Such *remaining population fraction*
 211 is thus

$$212 \quad \eta \equiv \frac{N_T}{N_T^\infty}, \quad (5)$$

213 where N_T and N_T^∞ are the total population sizes for finite and infinite habitat patches,
 214 respectively. We obtain these population sizes by integrating the population density over
 215 the entire landscape, including the matrix.

216 **3 Results**

217 **3.1 Perfectly absorbing matrix: the $r_M \rightarrow -\infty$ limit**

218 We first consider the simplest scenario in which individuals die instantaneously after they
 219 reach the habitat edges. In this limit, the population density is always zero in the matrix
 220 and, therefore, the movement component that biases individuals in the matrix toward the
 221 habitat edges is irrelevant. Movement is thus solely driven by random diffusion and the
 222 bias toward the attractive location $x = x_P = 0$. In large habitat patches, space-dependent
 223 movement leads to the accumulation of population density very close to regions with slower

224 movement. However, as the habitat patch decreases in size and regions with slower movement
 225 get closer to one of the habitat edges, the spatial pattern of population density changes due
 226 to mortality at the habitat edge and the maximum of population density shifts further away
 227 from the attractive location and towards the patch center (Fig. 2). This asymmetric pattern
 228 of space occupation due to space-dependent movement contrasts with well-known results for
 229 purely diffusive movement, for which population density reaches its maximum in the center
 230 of the habitat patch (Holmes et al., 1994), and significantly alters population loss because
 231 of habitat degradation.

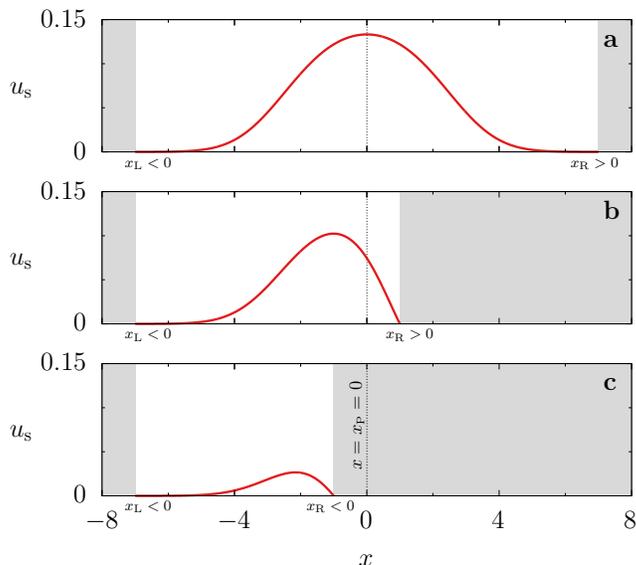


Figure 2: Stationary population density distribution $u_s(x)$ obtained from a numerical integration of Eq. 1. Space-dependence movement bias $v_p(x)$ is active and draws the population toward the attractive location $x = x_p = 0$. (a) $x_R = 7$ and $x_L = -7$, (b) $x_R = 1$ and $x_L = -7$, and (c) $x_R = -1$ and $x_L = -7$. Other parameters: $r_H = 0.1$, $\gamma = 1$, $D = 0.1$, $x_P = 0$, and $\tau_P^{-1} = 0.05$. Also, $r_M \rightarrow -\infty$. Gray regions represent the matrix.

232 First, to understand population loss due to habitat degradation, we use the remaining
 233 population fraction, η , defined in Eq. (5). This remaining population fraction is maximal
 234 when the attractive location is at the same distance from the two habitat edges, and it
 235 decays symmetrically about the line $x_R = -x_L$. Moreover, this decay is sharper for stronger
 236 bias toward the attractive location (Fig. 3 and S1). Finally, when the distance between
 237 the attractive location and one of the habitat edges is sufficiently large, further increasing
 238 the habitat size does not change the remaining population fraction because population loss
 239 through habitat edges is negligible, except for $\tau_P^{-1} = 0$.

240 Regarding the critical patch size, when the bias to the attractive location is strong,
 241 represented by higher values of τ_P^{-1} , the population is localized around the attractive location
 242 $x_P = 0$, and it goes extinct when the attractive location is within the habitat patch but close
 243 to one of its edges (Fig. 3a, b). When the bias to the attractive location decreases, however,
 244 the population can survive even if the attractive location is outside the habitat and the
 245 mortality in the matrix is infinite (Fig. 2c and 3c). This scenario would correspond to a

246 situation where habitat destruction places the attractive location outside the habitat and
 247 individuals have not adapted their movement behavior to this landscape modification. As
 248 a result, individuals preferentially move toward regions with low habitat quality, which can
 249 be understood as an example of an ecological trap (Lamb et al., 2017; Robertson and Hutto,
 250 2006a; Weldon and Haddad, 2005).

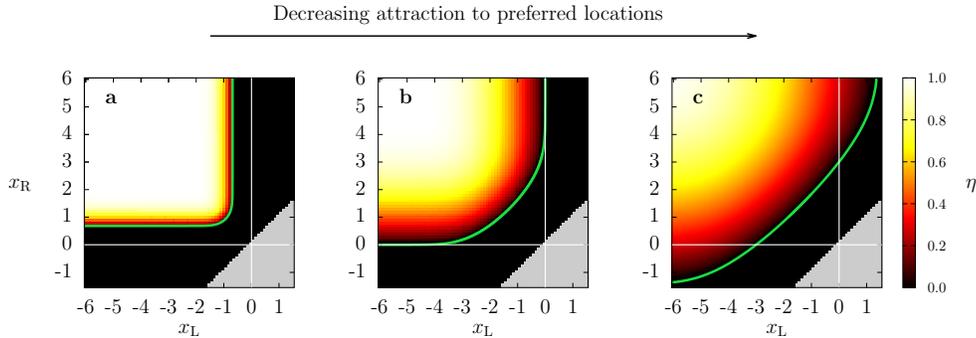


Figure 3: Remaining population fraction, η , for different habitat configurations (x_L, x_R) . (a) $\tau_P^{-1} = 0.5$, (b) $\tau_P^{-1} = 0.1$, and (c) $\tau_P^{-1} = 0.05$. Other parameters: $r_H = 0.1$, $D = 0.1$, and $\gamma = 1$. Also, $r_M \rightarrow -\infty$. The solid green line shows the critical patch size obtained with the semi-analytical method.

251 To further investigate how the distance between the attractive location and the habitat
 252 edges determines the critical patch size for different movement parameters, we calculate the
 253 critical location of the right habitat edge $x_{R,C}$ assuming that the left habitat edge is fixed and
 254 far from the attractive location. In these conditions, if x_R is also large, mortality through
 255 the left edge is negligible, but it becomes significant for smaller habitat patches. This setup
 256 mimics a situation where an initially large patch shrinks due to continued habitat destruction,
 257 slowly enough that the population distribution is at equilibrium for each particular
 258 habitat configuration, until it reaches a critical size and the population collapses. We find
 259 that the critical patch size is a nontrivial function of the intensity of the movement bias
 260 toward the attractive location and the distance between habitat edges and the attractive
 261 location. When $\tau_P^{-1} = 0.1$, $x_{R,C} = 0$ regardless of the value of D .

262 For $\tau_P^{-1} > 0.1$, movement bias is so strong that the attractive location must be within
 263 the habitat patch to avoid individuals entering the matrix and dying at a rate that cannot
 264 be outbalanced by population growth within the habitat (red region in Fig. 4 and Fig. S2).
 265 Moreover, due to strong bias toward the attractive location, the population is concentrated
 266 around that location. Increasing the diffusion coefficient D makes $x_{R,C}$ increase because the
 267 population spreads out, and individuals become more likely to reach the matrix and die.
 268 Increasing τ_P^{-1} from $\tau_P^{-1} = 0.1$ for a fixed diffusion coefficient D , we find a non-monotonic
 269 relationship between $x_{R,C}$ and τ_P^{-1} . First, the critical patch size increases with τ_P^{-1} because
 270 the population concentrates around the attractive location and are more likely to reach the
 271 matrix and die. For even higher attraction rate, the population concentrates very narrowly
 272 around the attractive location and individuals do not reach the habitat edge. As a result,
 273 the critical patch size decreases with τ_P^{-1} .

274 For $\tau_P^{-1} < 0.1$, $x_{R,C}$ is negative, which means that the population can persist even when

275 the attractive location is in the matrix (blue region in Fig. 4). In this low- τ_P^{-1} regime, $x_{R,C}$
 276 increases with τ_P^{-1} because less random movement increases the relative contribution of the
 277 movement bias to the population flux through the edge. Similarly, the critical patch size
 278 decreases with increasing D for values of τ_P^{-1} not too far from $\tau_P^{-1} = 0.1$. This negative cor-
 279 relation between critical patch size and diffusion appears because a more random movement
 280 reduces the tendency of individuals to cross the habitat edge (see Fig. S2b for curves of $x_{R,C}$
 281 versus D with fixed τ_P^{-1}). This phenomenon, known as the "drift paradox," has been pre-
 282 viously observed in organisms inhabiting streams, rivers, and estuaries where downstream
 283 drift is continuously present and extinction is inevitable in the absence of diffusion (Pachep-
 284 sky et al., 2005; Speirs and Gurney, 2001). However, as D continues to increase and random
 285 diffusion dominates dispersal, the critical patch size increases due to population loss via dif-
 286 fusion through both habitat edges. Finally, for very low values of τ_P^{-1} , diffusion controls the
 287 population flux through habitat edges and the behavior of the critical patch size converges
 288 to the theoretical prediction of the purely diffusive case, $L_C^D = \pi\sqrt{D/r_H}$ (Kierstead and
 289 Slobodkin, 1953).

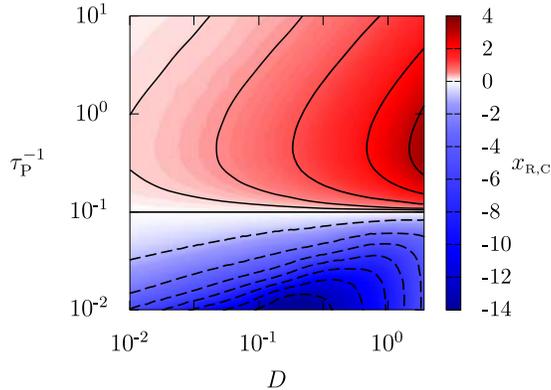


Figure 4: Critical location of the right habitat edge $x_{R,C}$ as a function of τ_P^{-1} and D . Parameter values: $r_H = 0.1$, $\gamma = 1$, $x_L = -20$, $r_M \rightarrow -\infty$.

290 3.2 Partially absorbing matrix and the effect of matrix-to-habitat bias

291 Considering finite r_M allows us to investigate how changes in movement behavior, once
 292 individuals reach the matrix, can alter the spatial pattern of population density and the
 293 critical patch size. If individuals in the matrix do not tend to return to the habitat ($\tau_M^{-1} \approx 0$),
 294 the population density decays into the matrix exponentially, and the critical patch size
 295 increases with matrix mortality rate (Fig. 5; Ludwig et al. 1979, Ryabov and Blasius 2008).

296 For low values of τ_M^{-1} , the tendency to return from the matrix to the habitat edges
 297 reduces how much the population penetrates the matrix and increases the population density
 298 inside the habitat, especially close to the edges (Fig. 5a). The spatial distribution of the
 299 population has a skewness that reaches its maximum when the attractive location is in
 300 the matrix (Fig. 5b). For large enough τ_M^{-1} , we observe that the edges act as almost hard
 301 walls. This would be equivalent to having reflecting boundary conditions. In this limit, the
 302 population survives for any habitat size (Maciel and Lutscher, 2013).

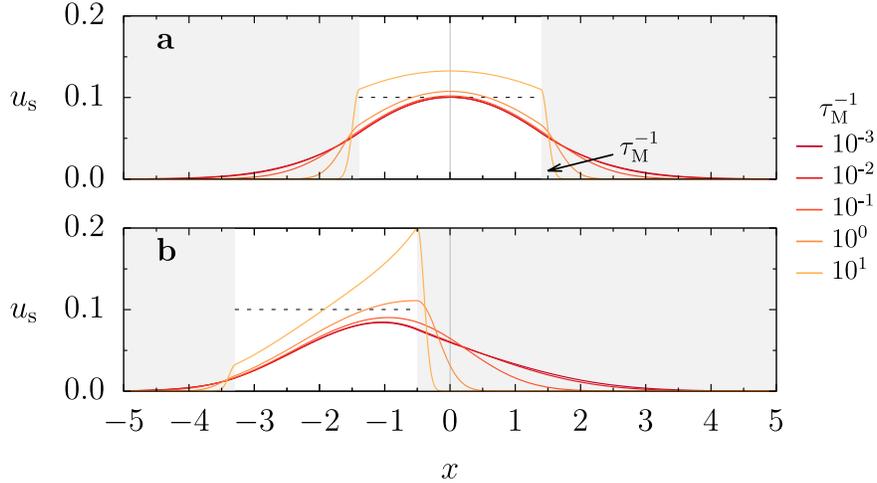


Figure 5: Stationary population density distribution $u_s(x)$ for the scenario with matrix-to-habitat attraction and attraction to the preferred location $x = x_P = 0$. The parameters are $L = 2.8$, which is smaller than the L_C for $r_M \rightarrow -\infty$, $\tau_P^{-1} = 0.05$, $r_M = -10^{-3}$, and τ_M^{-1} increasing for lighter colors, as indicated. (a) $x_R = -x_L = 1.4$ and (b) $x_R = -0.5$ and $x_L = -3.3$. Other parameters as in Fig. 2. In both panels, the dashed line corresponds to $u_s = r/\gamma$, which is the density inside the habitat for $\tau_M^{-1} \rightarrow \infty$ and $\tau_P^{-1} = 0$, in which case $u_s = 0$ in the matrix.

303 The accumulation of individuals around habitat edges suggests a potential tradeoff be-
 304 tween a decrease in mortality in the matrix due to the attraction to habitat edges and an
 305 increase in intraspecific competition due to higher population densities in the habitat. To
 306 investigate the impact of this tradeoff on population loss due to habitat degradation, we
 307 measure the fraction of the population that remains for a given patch size relative to the
 308 value for an infinite habitat patch, η . We perform this measurement for several values of
 309 the matrix mortality rate r_M and the returning rate to habitat edges τ_M^{-1} , which are the two
 310 main parameters controlling the accumulation of population density at habitat edges. We
 311 consider a scenario with the attractive location at the center of the habitat patch, which is
 312 the limit where we have a weaker accumulation of individuals at habitat edges and, there-
 313 fore, the regime in which the tradeoff between matrix mortality and intraspecific competition
 314 around habitat edges has a weaker effect on population dynamics.

315 At high matrix mortality rates, the population does not survive ($\eta = 0$), except for very
 316 high returning rates τ_M^{-1} (Fig. 6). When the matrix mortality rate decreases, η increases
 317 and remains a monotonically increasing function of τ_M^{-1} . For r_M closer to zero, however, η
 318 becomes a non-monotonic function of τ_M^{-1} . For these values of the matrix mortality rate,
 319 increasing the returning rate to habitat edges is initially detrimental to the total population
 320 size because it leads to higher intraspecific competition at the habitat edges, which outweighs
 321 the decrease in mortality in the matrix. In other words, the density distribution does
 322 not penetrate the matrix as far (Fig. 5a) while, inside the habitat, competition does not
 323 allow for a large enough increase in population, and so the total population decreases.
 324 Consequently, the habitat edge itself behaves as an ecological trap in this regime, and our
 325 model recovers a behavior similar to previous observations for insects (Ries and Fagan,
 326 2003; Ries et al., 2004). Above a critical value of τ_M^{-1} at which η is minimal, further

327 increasing the returning rate to habitat edges becomes beneficial for population persistence
 328 because now very few individuals enter the matrix and reduced matrix mortality outweighs
 329 the increased intraspecific competition at habitat edges. For infinite return rate τ_M^{-1} , all
 330 the curves for different values of the matrix mortality rate r_M converge to the same value
 331 because individuals do not penetrate the matrix. For $\tau_M^{-1} \rightarrow \infty$ and $\tau_P^{-1} = 0$, one has
 332 $u_s = r/\gamma$ inside the habitat and $u_s = 0$ in the matrix (dashed line in Fig. 5). The existence
 333 of a non-monotonic dependence of population size on advection strength is reminiscent of a
 334 behavior reported in a different scenario for a model with advection towards a continuous
 335 environmental gradient (Belgacem and Cosner, 1995).

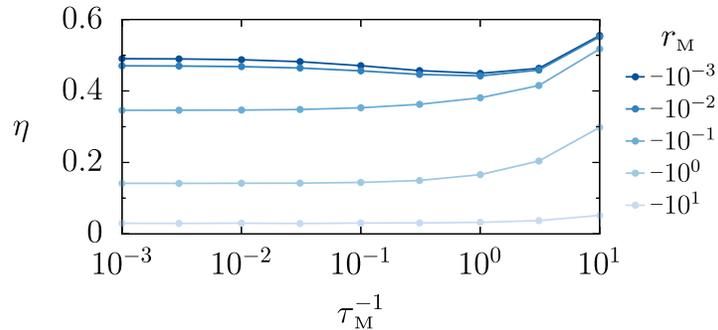


Figure 6: Ratio between the total population for L and for $L \rightarrow \infty$, η , versus τ_M^{-1} .
 $x_R = -x_L = 1.4$ and values of r_M as indicated, with lighter colors corresponding to larger absolute
 values of r_M . Other parameters as in Fig. 5.

336 4 Discussion

337 We studied the spatial dynamics of a population in a finite habitat surrounded by an infi-
 338 nite matrix, considering different ratios between matrix mortality and habitat reproduction
 339 rates. We additionally incorporated space-dependent deterministic movement through an
 340 advection term that attracts individuals toward specific landscape locations, including habi-
 341 tat edges. This advection term can create spatial distributions of population density that
 342 are asymmetric with respect to the center of the patch, especially when the patch size is
 343 small and attractive regions lie near habitat edges. This result could explain why, in cer-
 344 tain species, populations tend to accumulate in the periphery of the species historical range
 345 following geographical range contraction (Channell and Lomolino, 2000a,b). Moreover, our
 346 results show that both the habitat carrying capacity and critical size depend nonlinearly,
 347 sometimes non-monotonically, on movement and demographic parameters and the location
 348 of the habitat edges relative to regions of slower movement. Recent work has also found
 349 nonlinear and non-monotonic relationships between movement and landscape parameters
 350 underlying the stability of prey-predator systems in fragmented landscapes (Dannemann
 351 et al., 2018; Nauta et al., 2022). These findings emphasize the importance of untangling the
 352 various contributions determining individual movement, including environmental covariates,
 353 when designing conservation strategies such as refuges in fragmented landscapes or marine
 354 protected areas (Gaston et al., 2002; Gerber et al., 2003).

355 Specifically, for very low yet non-zero bias intensities, we find a range of values for the
356 diffusion coefficient for which the critical habitat size decreases with increasing diffusion.
357 This counterintuitive phenomenon is known as the “drift paradox” (Pachepsky et al., 2005).
358 On the opposite limit, if movement bias toward the attractive location is very strong, the
359 population becomes ultra-localized and its survival depends on whether the attractive site
360 is in the habitat patch or the matrix; if it is in the patch, the population will persist, but if
361 it is in the matrix, the population will go extinct. In between these two limits, for weak bias
362 toward the attractive location, further increasing bias intensity increases the critical habitat
363 size when the attractive site is inside the habitat but not too far from both edges. Moreover,
364 populations are still viable for these weak bias intensities even if habitat destruction places
365 the attractive location inside the matrix, creating an ecological trap. Ecological traps are
366 often related to human landscape interventions (Robertson and Hutto, 2006b; Schlaepfer
367 et al., 2002) such as the construction of bird nest cavities in regions with generally worse
368 conditions than those where the birds would naturally build their nests (Krams et al., 2021).
369 Roads can also act as ecological traps. For example, female bears with their cubs are often
370 attracted to roads due to higher forage availability and to avoid potential male infanticide,
371 increasing their risk of being killed in vehicle collisions (Northrup et al., 2012; Penteriani
372 et al., 2018).

373 Our model also suggests that movement responses to changes in habitat quality, such
374 as the tendency of individuals to return from the matrix to habitat edges, can result in the
375 accumulation of population density around habitat edges, even when attractive locations
376 are centered in the habitat patch. This accumulation of population density reduces the
377 quality of regions nearby habitat edges relative to the surrounding matrix and turn the
378 neighborhoods of habitat edges into ecological traps. This population crowding nearby
379 habitat edges could, however, be eliminated by density-dependent dispersal, which was
380 not included in the our model. Animal responses to changes in habitat fragmentation,
381 such as the matrix avoidance term included in our model, might be relevant in regulating
382 demographic responses to habitat destruction. Quantifying correlations between movement
383 behavior, habitat quality, and population density in animal tracking data could help to
384 understand the impact of further habitat destruction on population viability. More generally,
385 the existence of ecological traps suggests that movement patterns exhibited by individuals
386 upon habitat destruction do not correspond to an evolutionarily stable strategy (Hastings,
387 1983). However, because ecological traps do not necessarily lead to population extinctions
388 in our model, individuals could potentially adapt their movement behavior to avoid newly
389 degraded regions.

390 Different non-uniform space utilization patterns and preference for specific habitat loca-
391 tions are ubiquitous in nature. We consider that all individuals in the population have the
392 same movement behavior and thus share habitat preferences. This assumption is an accurate
393 modeling choice for certain species, such as central-place foragers (Fagan et al., 2007). Very
394 often, however, habitat preferences vary across individuals in a population, which might im-
395 pact how individuals interact with one another (Martinez-Garcia et al., 2020; Noonan et al.,

396 2021). Incorporating individual-level variability in space utilization would inform how pop-
397 ulations of range-resident and territorial species would respond to habitat destruction, and
398 is one of the future directions that could be explored based on this work. However, while at-
399 tractiveness can sometimes be quantified in terms of environmental covariates (Mueller et al.,
400 2008) or by knowing the locations of landscape features like watering holes, other times it
401 will be difficult or impossible to quantify, for example when “attractiveness” depends on the
402 unknown distribution of a particular prey species. Future theoretical research should aim to
403 increasingly fill this gap between existing models describing empirically observed patterns
404 of animal movement and higher level ecological processes.

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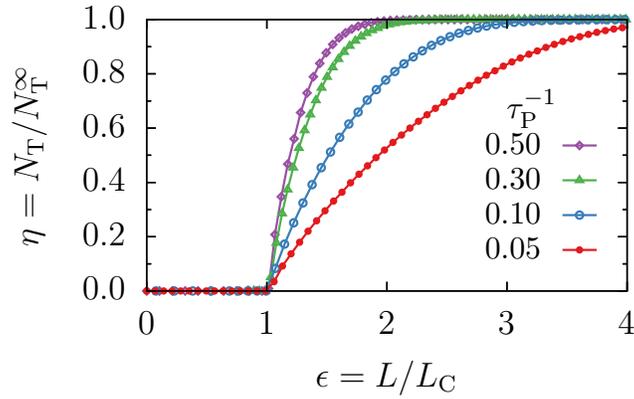


Figure S1: Ratio between the total population for L and for $L \rightarrow \infty$, η , versus $\epsilon \equiv L/L_C$ for various τ_P^{-1} as indicated. Other parameters: $D = 0.1$, $\gamma = 1$, $r_H = 0.1$, and $r_M \rightarrow -\infty$. The habitat is symmetric, i.e., $x_R = -x_L$.

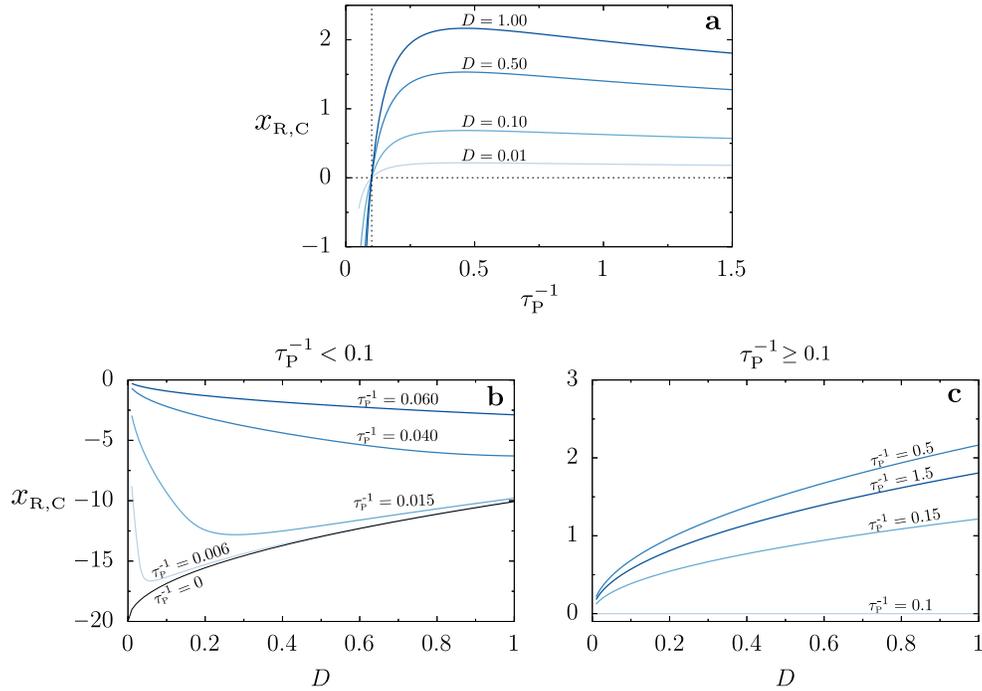


Figure S2: Critical location of the right habitat edge $x_{R,C}$ (a) as a function of τ_P^{-1} , and as a function of D for (b) $\tau_P^{-1} < 0.1$ and (c) $\tau_P^{-1} > 0.1$. Other parameters: $r_H = 0.1$, $\gamma = 1$, $r_M \rightarrow -\infty$, and $x_L = -20$.