Spring College in the Physics of Complex Systems | (SMR 4207)

16 Feb 2026 - 13 Mar 2026
ICTP, Trieste, Italy

P01 - ABDELAZIZ Gehad Saber Saber

COMPUTATIONAL STUDY OF THE INTERACTION BETWEEN GRP78 AND THE ENGINEERED EGF-SUBA CHIMERIC PROTEIN FOR TARGETED CANCER THERAPY

P02 - SAKAM ABO Esaie

Stochastic Optimal Control of differential equations using the maximum principle.

P03 - AGRAWAL Ramgopal

Disordered Baxter model: Lack of self-averaging and Multi-fractal behavior

P04 - ARSHADI KALEMEH Amirhossain

Modeling Enzyme Network Structure via Centrality Correlations

P05 - ANAND Amida

A Tale of Two Criticalities: How the Brain Learns through the lens of Criticality

P06 - ASHRAF Ashveed

Quantifying Consensus in Effective Model Inference for Disordered Ising Systems

P07 - CAAMANO Federico

Dark energy, physical and evolutionary frustration in ankyrin repeat proteins

P08 - DU Yao

Versatile reservoir computing for heterogeneous complex networks

P09 - FOTINOS Jeronimo

Stemness Percolation in Tumorspheres

P10 - FOUELIFACK NGUESSAP Ediline Laurence

Emergent Critical Dynamics Underlying Resilience and Collapse in Amyloid-Driven Neuronal Networks

P11 - FRIGERIO Giacomo

Chimera games emerging from coevolutionary dynamics with endogenous feedbacks

P12 - KIMATHI Godfrey Kariuki

Fuel-Driven Active Brownian Particles with Time-Dependent Propulsion

P13 - KUHN Adam Miles, Hipolito

Augur Network Facilitates Protein Discovery and Design

P14 - MARRA SOLAZZO Michela

SUPRA-LINEAR STORAGE IN DENSE NETWORKS OF GRID AND PLACE CELLS

P15 - MENUCI MUCCILLO Vinicius

Resource-mediated interactions shape spatial patterns in individual-based models of vegetation dynamics

P16 - MOHAMED Almostafa Adel Saad

Interplay of Hexatic Order and Hyperuniformity in Model Biological Tissues

P17 - MOLLINEDA RODRIGUEZ Amanda

Entropic Analysis of Cardiac Signals

P18 - PAYANDEH Fatemeh

The effect of flocking on the orientation of migratory species

P19 - RAFAT Mohammad Nasir

Investigating chimera states in dynamical networks with adaptive coupling

P20 - RAMOS AMBOU Lorena

Logical model for intracellular signaling in CD8+ T cells mediated by cytokines modulating the immune response.

P21 - ROZO LOZANO Camilo Andres

Information Flow and Fractional Diffusion in Networks (Flujo de información y difusión fraccionaria en redes)

P22 - SAFARPOURDOBAKHSHARY Aminreza

An Adaptive Q-Learning Controller for Microrobots in Dynamic Thermal Environments

P23 - TABASSUM RIYA Nowshin

Viability of Transition Metal-Doped Tin Nanotechnology as Biosensor Material for Neural Disorder Detection

P24 - TANGSONGCHAROEN Krit

CrystalGRW: Generative Modeling of Crystal Structures with Targeted Properties via Geodesic Random Walks

P25 - VARETTI Sara

The Architecture of Cortical Timing: From Local Clustering to Global Hierarchies

P26 - VILLACIS RAMON Jhon Steeven

Self-Control of Supertransient Collective Chaos in Coupled Map Networks

P27 - YARAHMADI Hediye

We model language evolution using 94 syntactic parameters, incorporating both implicational constraints and random, asymmetric interactions. Simulations with Glauber dynamics reveal glassy dynamics at low asymmetry and ongoing evolution at higher asymmetry, with a sharp transition around $\varphi = 30°$. Results suggest that disorder critically shapes slow, long-term syntactic change.

P28 - ZULQURNAIN Muhammad

SIMULATION OF FLUID DYNAMICS USING CFD, PHYSICS-INFORMED NEURAL NETWORKS, AND STOCHASTIC

P01

COMPUTATIONAL STUDY OF THE INTERACTION BETWEEN GRP78 AND THE ENGINEERED EGF-SUBA CHIMERIC PROTEIN FOR TARGETED CANCER THERAPY

Gehad Saber Ali Abd Elaziz[1], Abdo A. Elfiky[2], Yasser Y. Obeid[3]

[1] *Department of Physics, Faculty of Science, Fayoum University, Egypt*
[2] *Department of Biophysics, Faculty of Science, Cairo University, Egypt*
[3] *Department of Physics, Faculty of Science, Fayoum University, Egypt*

The molecular chaperone GRP78 is a central regulator of protein folding and cellular stress response, frequently overexpressed in tumor cells where it promotes survival and resistance to therapy. Its selective inhibition has emerged as a promising approach for sensitizing cancer cells to stress-induced death. The catalytic subunit of the Subtilase cytotoxin, SubA, specifically cleaves GRP78, leading to disruption of proteostasis and apoptosis. However, SubA lacks intrinsic selectivity for cancer cells.

To address this limitation, a chimeric protein (EGF-SubA) has been designed, in which epidermal growth factor (EGF) serves as a targeting ligand directing SubA to EGFR-overexpressing tumor cells. This study aims to explore the structural interaction between GRP78 and EGF-SubA using molecular docking and molecular dynamics simulations. The analysis focuses on identifying binding interfaces, evaluating complex stability, and characterizing conformational rearrangements upon binding.

The expected outcomes will provide detailed structural insights into the GRP78–EGF-SubA complex and clarify the molecular basis of selective targeting. These findings could guide the rational design of new targeted anticancer agents that combine receptor specificity with disruption of GRP78-mediated protective pathways, offering a potential strategy to overcome tumor resistance.

References

[1] *Chapter Three - Targeting the Unfolded Protein Response in Cancer Therapy*, Advances in Cancer Research, Vol. 140, 2018, pp. 69–94.
[2] *Chaperone-Targeting Cytotoxin and Endoplasmic Reticulum Stress-Inducing Drug Synergize to Kill Cancer Cells*, Scientific Reports, 2020, 10: 13502.

P02

Stochastic Optimal Control of differential equations using the maximum principle.

P03

Disordered Baxter model: Lack of self-averaging and Multi-fractal behavior

Ramgopal Agrawal[1], **Victor Dotsenko**[2], **Maxym Dudka**[3,4,5], **Marco Picco**[6], **Enzo Marinari**[1,7] **and Gleb Oshanin**[2]

[1]*Dipartimento di Fisica, Sapienza Università di Roma, Piazzale Aldo Moro 5, Rome, 00185, Italy*

[2]*Laboratoire de Physique Théorique de la Matière Condensée (UMR CNRS 7600), Sorbonne Université, 4 Place Jussieu, 75252 Paris, France*

[3]*Institute for Condensed Matter Physics, National Acad. Sci. of Ukraine, 79011 Lviv, Ukraine*

[4]*Doctoral College for the Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry* ($\mathbb{L}^4$)*, Europe*

[5]*Lviv Polytechnic National University, 79013, Lviv, Ukraine*

[6]*Laboratoire de Physique Théorique et Hautes Energies (UMR CNRS 7589), Sorbonne Université, 4 Place Jussieu, 75252 Paris, France*

[7]*INFN, Sezione di Roma 1 and Nanotech-CNR, UOS di Roma, P.le A. Moro 2, I-00185, Roma, Italy*

In this work, we investigate a weakly disordered Baxter eight-vertex model at the pseudo-critical point. In the critical region, the model is formulated in terms of interacting *Grassmann–Majorana* spinor fields with four-spin interactions and solved in the limit $|g_0| \ll 1$ using a combination of the replica method and renormalization-group techniques. We show that the relative variance of the critical internal energy approaches a constant value in the thermodynamic limit $L \to \infty$. Consequently, fluctuations are relevant, and both the internal energy and the free energy lack self-averaging, implying that many large samples are required to determine their actual values. Our analytical predictions are supported by numerical simulations on finite-dimensional lattices. Moreover, we find that the moments of the spatial correlation function exhibit strong multifractal behavior.

P04

Modeling Enzyme Network Structure via Centrality Correlations

Arshadi, Amirhossain[1]; Tabatabaei, Mohammad[1]; Shahbazi, Farhad[1]

[1] *Department of Physics, Isfahan University of Technology, Isfahan*

In this study, the correlation matrix of centrality measures is employed as a tool to reveal the internal structure and topological features of Enzymes' networks. Based on this, it is also used as a metric to quantify the similarity between networks. The aim is to reconstruct this correlation matrix using three classical network generation models, while preserving the fundamental properties of the Enzyme networks. The results indicate that the Watts–Strogatz[1] model offers a better fit in reproducing the centrality correlation [2] patterns, although the match is still not perfect. Accordingly, we propose directions for future research focused on developing hybrid models to improve the accuracy of centrality correlation reconstruction.

Network	N	E	Deg	Clus	Dens	Rad	Diam	Best Fit (*)	BA Diff	WS Diff	ER Diff	Deg*	Clus*	Rad*	Diam*
g1	37	84	4.54	0.565	0.126	6	12	WS	20.51	9.87	19.93	4.00	0.386	4.62	7.05
g10	32	53	3.31	0.601	0.107	10	19	WS	21.62	8.52	19.25	2.00	0.003	11.21	21.23
g101	45	88	3.91	0.281	0.089	8	15	WS	21.70	11.28	20.13	4.00	0.387	5.02	7.70
g102	42	82	3.90	0.239	0.095	7	14	WS	18.64	8.22	17.26	4.00	0.384	4.89	7.51
g103	59	115	3.90	0.235	0.067	7	13	WS	19.75	8.54	18.73	4.00	0.384	5.57	8.70
g113	52	98	3.77	0.205	0.074	8	16	WS	25.09	14.59	23.86	4.00	0.379	5.28	8.15
g123	90	127	2.82	0.105	0.032	9	12	BA	6.20	9.57	6.62	1.98	0.000	5.35	10.21
g13	42	75	3.57	0.559	0.087	12	23	WS	21.78	11.09	20.22	4.00	0.386	4.87	7.49
g183	42	94	4.48	0.345	0.109	5	9	WS	9.99	4.15	9.33	4.00	0.386	4.94	7.54
g199	62	108	3.48	0.162	0.057	13	26	WS	12.55	2.52	11.35	2.00	0.002	18.98	36.93

Table 1: Comparison of structural features of enzyme interaction networks with different models

[1] A. Author, B. Coauthor, J. Sci. Res. **13**, 1357 (2012).
[2] A. Author, B. Coauthor, J. Sci. Res. **17**, 7531 (2013).

P05

A Tale of Two Criticalities: How the Brain Learns through the lens of Criticality

Amida Anand
Imperial College London

In recent years, a growing body of evidence suggests that the brain operates near a critical point, balancing order and disorder to optimise computation, memory, and adaptability. Although empirical studies have identified critical signatures on spatial and temporal scales, a systematic framework remains underdeveloped and insufficiently formalised. This thesis addresses this gap and introduces a dual-probe framework that begins to unite these perspectives, using Artificial Neural Networks (ANNs) as proxies for biological learning.

Structural criticality is quantified by mapping network weights to effective spin couplings and computing the critical temperature (T_c), a measure of attractor stability. Temporal criticality is quantified by fitting autoregressive models to population dynamics and measuring distance (d_2) from the $\beta = 2$ hyperplane, a marker of critical slowing down. Across training, T_c increased monotonically, indicating consolidation, while d_2 exhibited a triphasic trajectory: early dip, mid-training rise, and late decline. Noise and forgetting perturbations revealed distinct divergences between the two probes.

Taken together, these results highlight the existence of dual criticality in learning: structural consolidation drives systems away from criticality, while temporal adaptability preserves near-critical dynamics. This reconciles long-standing tensions between attractor stability and avalanche-like flexibility and provides a mathematical account of the confusion-to-understanding shift, laying the foundations for a general principle.

[1] P. Bak, C. Tang, and K. Wiesenfeld, “Self-organized criticality: An explanation of the 1/f noise,” Physical Review Letters, vol. 59, no. 4, pp. 381–384, Jul. 27, 1987
[2] D. R. Chialvo, “Critical brain networks,” Physica A: Statistical Mechanics and its Applications, Complexity and Criticality: in memory of Per Bak (1947–2002), vol. 340, no. 4, pp. 756–765, Sep. 15, 2004
[3] J. M. Beggs and D. Plenz, “Neuronal avalanches in neocortical circuits,” Journal of Neuroscience, vol. 23, no. 35, pp. 11 167–11 177, Dec. 3, 2003
[4] J. M. Beggs, “The Cortex and the Critical Point: Understanding the Power of Emergence”, The MIT Press, Aug. 30, 2022
[5] J. Fontenele, N. A. P. de Vasconcelos, T. Feliciano, et al., “Criticality between cortical states,” Physical Review Letters, vol. 122, no. 20, p. 208 101, May 21, 2019

P06

Quantifying Consensus in Effective Model Inference for Disordered Ising Systems

Ashveed Ashraf[1]

[1]Department of Chemistry, Gandhi Institute of Technology and Management (GITAM) University, Bengaluru, India

Inferring reliable and self-consistent models from disordered data is challenging, as limited and noisy observation often cause different learners to arrive at conflicting descriptions of the same underlying structure. We define *consensus* as the degree to which independently trained learners agree on a shared effective model, which provides a quantifiable measure of reliability under disorder and finite data. To formalize this, we present consensus learning, a method for assessing the stability of inferred models by studying a teacher-student model [1] setup on the disordered 2D Ising model. The teacher creates Monte Carlo samples with quenched disorder, and an ensemble of students, for each given data from a fixed disorder realization, infer a uniform effective coupling J^* by fitting a flexible kernel logistic model [2] and then projecting it onto a uniform interaction. Aggregating the inferred coupling over several students and disorder realizations yields the consensus distribution $P(J^*)$, which reflects the reliability and agreement of inference across disorder.

We analyze the width of the consensus distribution $P(J^*)$ as a learning based diagnostic for self averaging in disordered systems, asking how consistently different learners can agree on a uniform effective coupling across disorder realizations. Within this framework, we study how consensus varies with temperature and disorder strength, as well as whether inferred couplings reveal criticality or non self-averaging signs. For evaluating the information retained by a uniform effective model, we calculate the structure lost during the compression phases using residual complexity. We evaluate the kernel-to-projection pipeline and simple uniform fitting to determine which approach produces more stable and less biased results across various disorder regimes.

This approach makes consensus learning a systematic tool for investigating model misspecification, calculating self-averaging, and determining the constraints of effective descriptions in disordered statistical systems. It also brings together statistical physics and modern learning theory by illustrating how disorder and criticality impact not just physical observables but also the stability and consistency of successful models inferred by different learners.

References

[1] B. Loureiro, C. Gerbelot, H. Cui, S. Goldt, F. Krzakala, M. Mézard, and L. Zdeborová, Adv. Neural Inf. Process. Syst. **34**, 18137 (2021).

[2] J. Zhu and T. Hastie, Adv. Neural Inf. Process. Syst. **14**, 1081 (2001).

P07

Abstract template for poster “Dark energy, physical and evolutionary frustration in ankyrin repeat proteins”

Federico Caamaño [1] **and Diego U. Ferreiro** [1]

[1] *Protein Physiology Lab, Departamento de Química Biológica, Universidad de Buenos Aires, Instituto de Química Biológica de la Facultad de Ciencias Exactas y Naturales (IQUIBICEN-CONICET), Buenos Aires, Argentina*

Evolution shapes protein sequences by preserving mutations that maintain function, thereby creating evolutionary constraints. These constraints manifest as position-specific amino acid frequencies and correlations between contacting residues. Direct-Coupling Analysis (DCA) uses multiple sequence alignments to derive an evolutionary force field (comprising local fields and pairwise couplings) that assigns an effective energy to sequences.

According to energy landscape theory, proteins must minimize energetic frustration to fold efficiently. Native frustration correlates with function and can be measured experimentally or via force fields such as AWSEM. Similarly, evolutionary frustration can be computed using DCA derived energies.

We introduce “Dark Energy” as the difference between the mutational perturbations in the folding and evolutionary energy landscapes. This metric helps localize and quantify evolutionary constraints.

We analyzed 300 ankyrin repeat proteins, computing physical frustration, evolutionary frustration, and Dark Energy to map evolutionary constraints in this family, comparing the established local frustration method with the novel Dark Energy approach.

[1] JD. Bryngelson, JN. Onuchic, ND. Socci, PG. Wolynes. Funnels, pathways, and the energy landscape of protein folding: A synthesis. Proteins. (1995).
[2] EA. Galpern, J. Marchi, T. Mora, AM. Walczak, DU. Ferreiro. Evolution and folding of repeat proteins. Proc Natl Acad Sci USA. (2022)
[3] DU. Ferreiro, EA. Komives, PG. Wolynes. Frustration, function and folding. Current Opinion in Structural Biology. (2018)
[4] S. Cocco, C. Feinauer, M. Figliuzzi, R. Monasson, M. Weigt. Inverse statistical physics of protein sequences: a key issues review. Rep Prog Phys. (2018)
[5] R. Espada, RG. Parra, T. Mora, AM. Walczak, DU. Ferreiro. Inferring repeat-protein energetics from evolutionary information. AV. Morozov, editor. PLoS Comput Biol. (2017)
[6] EA. Galpern, C. Bueno, IE. Sánchez, PG. Wolynes, DU. Ferreiro. Probing the Dark Energy in the Functional Protein Universe. Arxiv (2025).

P08

Versatile reservoir computing for heterogeneous complex networks

P09

Stemness Percolation in Tumorspheres

J. Fotinós[1,2], **C. A. Condat**[1,2], **L. Vellón**[3], **and L. Barberis**[1,2]

[1]*Faculty of Mathematics, Astronomy, Physics, and Computing, National University of Córdoba, Argentina*
[2]*Enrique Gaviola Institute of Physics, CONICET, Argentina*
[3]*Stem Cells Lab, IBYME, CONICET, Buenos Aires, Argentina*

Cancer stem cells (CSCs) are believed to sustain tumor growth and contribute to relapse and therapy resistance. Tumorsphere cultures provide a convenient in vitro model to study CSC behavior and spatial organization.

We develop a theoretical model for tumorsphere growth that highlights mechanisms linked to invasive potential. In particular, we evaluate the probability of finding CSCs at the spheroid surface, since these may detach without undergoing anoikis, a form of programmed cell death, and thus initiate invasion. By treating stemness as a transferable, diffusing trait on a directed space–time graph, we establish an analogy with percolation theory and compute the corresponding critical probability for CSC propagation. Remarkably, this critical probability equals 1, indicating that percolation is effectively one-dimensional even in n-dimensional systems. This suggests that CSCs eventually become confined to the spheroid interior, implying that invasion must occur early during growth or rely on additional symmetry-breaking factors enhancing invasive potential.

With experiments in mind, we perform numerical simulations of 3D spheroids to verify the predicted critical probability and examine finite-size effects. The simulations further characterize the spatial distribution of CSCs predicted by the model, revealing a strongly non-homogeneous pattern.

To assess our model's predictions and, in particular, the departure from well-mixed assumptions in classical ODE formulations [1], we conduct experiments on tumorspheres enriched in CSCs. SOX2 expression, a marker indicating stemness, is detected by confocal microscopy, and a dedicated image-analysis pipeline integrating clustering and computer-vision methods is used to localize and quantify CSCs within spheroids [2].

Taken together, the experimental results confirm a spatially heterogeneous arrangement of CSCs, consistent with our simulations and with the predictions of the percolation-based framework.

[1] J. Fotinós, L. Barberis, C.A. Condat, "Effects of a differentiating therapy on cancer-stem-cell-driven tumors", *J. Theor. Biol.* **572**, 111563 (2023).
[2] J. Fotinós, M.P. Marks, L. Barberis, L. Vellón, "Assessing the distribution of cancer stem cells in tumorspheres", *Sci. Rep.* **14**, 11013 (2024).

P10

Abstract template for Emergent Critical Dynamics Underlying Resilience and Collapse in Amyloid-Driven Neuronal Networks

Ediline L. F. Nguessap[1], **Fernando F. Ferreira**[1]

[1]*Department of Physics,FFCLRP-University of Sao Paulo, 14040900, Ribeirao Preto-SP, Brazil*

Alzheimer's disease involves progressive synaptic degradation that ultimately disrupts large-scale brain connectivity, yet the dynamical route from local pathology to global collapse remains unclear. Here, we introduce a multiscale computational framework that integrates small-world network topology [1], Izhikevich neuronal dynamics [2], short-term synaptic plasticity, and amyloid-β–induced synaptic pruning to explore how functional brain networks lose resilience under pathological stress.

Using principles from nonlinear dynamics and complex systems theory [3], we uncover a biphasic evolution of network dynamics. An initial compensatory regime preserves synchronization and efficiency despite progressive degradation, followed by a critical transition beyond an amyloid threshold [5, 4] that triggers a rapid collapse of global connectivity. Notably, early-warning indicators such as declining global efficiency and rising spike entropy precede the structural breakdown, revealing the onset of dynamical instability [3].

These results provide a quantitative link between amyloid accumulation, network topology, and collective neural activity, establishing phase-like transitions as a unifying framework to describe resilience loss in Alzheimer's disease [6].

Keywords: Complex systems; Critical transitions; Resilience; Amyloid-β; Alzheimer's disease

[1] D. S. Bassett and E. Bullmore, Neuroscientist **12**, 512 (2006).
[2] E. M. Izhikevich, IEEE Trans. Neural Netw. **14**, 1569 (2003).
[3] M. Scheffer, S. R. Carpenter, T. M. Lenton, J. Bascompte, W. Brock, V. Dakos, J. Van de Koppel, I. A. Van de Leemput, S. A. Levin, and E. H. Van Nes, Science **338**, 344 (2012).
[4] C. R. Jack Jr, D. A. Bennett, K. Blennow, M. C. Carrillo, B. Dunn, S. B. Haeberlein, D. M. Holtzman, W. Jagust, F. Jessen, J. Karlawish *et al.*, Alzheimer's Dement. **14**, 535 (2018).
[5] W. J. Jagust and S. M. Landau, Neurology **96**, e1347 (2021).
[6] R. S. L. Chia, K. Minta, L.-Y. Wu, K. H. T. Salai, Y. L. Chai, S. Hilal, N. Venketasubramanian, C. P. Chen, J. R. Chong, and M. K. P. Lai, Biomolecules **14**, 75 (2024).

P11

Chimera games emerging from coevolutionary dynamics with endogenous feedbacks

Federico M. Quetti[1], Andrea Civilini [2,6,8], Giacomo Frigerio[8], Silvia Figini[9] , Giacomo Livan[3,4,5], Vito Latora[2,7,8]

[1]*Dipartimento di Matematica, Università di Pavia, Via Ferrata 5, 27100 Pavia, Italy*
[2]*School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom*
[3] *Dipartimento di Fisica, Università di Pavia, Via Bassi 6, 27100 Pavia, Italy*
[4] *Department of Computer Science, University College London, 66-72 Gower Street, WC1E 6EA London, United Kingdom*
[5] *INFN, Sezione di Pavia, Via Bassi 6, 27100 Pavia, Italy*
[6] *Sorbonne Université, Paris Brain Institute (ICM), CNRS UMR7225, INRIA Paris, INSERM U1127, Hôpital de la Pitié Salpêtrière, AP-HP, Paris 75013, France*
[7] *Complexity Science Hub Vienna, A-1080 Vienna, Austria*
[8] *Dipartimento di Fisica ed Astronomia, Università di Catania and INFN, Catania I-95123, Italy*
[9] *Dipartimento di Scienze Politiche e Sociali, Universit'a di Pavia, 27100 Pavia, Italy*

From climate change to financial bubbles and wars, the accelerating pace of global change reveals that the commonly adopted assumption of a static environment in evolutionary game-theoretic models is often unrealistic. In this work, we introduce a coevolutionary game framework in which strategy dynamics and environmental feedbacks evolve in mutual dependence. Specifically, the game played at any time is endogenously defined as a convex combination of two social dilemmas, weighted by the instantaneous abundance of cooperators in the population. This minimal feedback mechanism gives rise to a rich phenomenology: depending on the choice of the underlying social dilemmas, qualitatively distinct dynamical regimes—denoted as **Chimera games** —emerge. In these games, the equilibrium level of cooperation can become unstable under standard evolutionary dynamics, despite identical payoff structures, while under alternative feedback couplings, previously unstable equilibria may instead stabilize. Such behaviour challenges the conventional view that equilibrium properties are solely determined by fixed payoff matrices and highlights the importance of endogenous feedbacks in shaping collective dynamics.

Our findings suggest that even simple forms of coevolutionary coupling between strategies and payoffs can drastically alter the stability landscape of social dilemmas. This has profound implications for the predictability and control of social and ecological systems, where interventions based only on instantaneous system states may yield counterintuitive outcomes.

[1] Quetti, Federico Maria and Civilini, Andrea and Frigerio, Giacomo and Figini, Silvia and Livan, Giacomo and Latora, Vito, arXiv preprint arXiv:2506.20603 (2025).
[2] Weitz, Joshua S., Eksin, Ceyhun, Paarporn, Keith, Brown, Sam P., and Ratcliff, William C., Proceedings of the National Academy of Sciences, 113(47), E7518–E7525 (2016).
[3] Tilman, Andrew R., Plotkin, Joshua B., and Akçay, Erol, Nature Communications, 11(1), 915 (2020).

P12

Fuel-Driven Active Brownian Particles with Time-Dependent Propulsion

Godfrey kariuki[1], T.B Liverpool[2], and R.Hawkins[3]

Active matter systems consist of self-driven particles that continuously consume energy to generate directed motion. These systems exhibit complex collective behaviours, such as pattern formation, phase separation, and anomalous transport, and are usually exhibited through micron-scale active colloids. In this work, a recently developed theoretical framework for non-equilibrium statistical mechanics is applied to computational models of active colloids. Our goal is to examine emergent phenomena in self-propelled particle systems through extensive molecular dynamics simulations and compare them to simulation findings and theoretical predictions. The study advances our knowledge of how rich macroscopic dynamics arise from sustained energy input at the microscopic scale.

[1] Sasamoto, T. and Spohn, H. Phys. Rev. Lett. 104(23), 230602 jun (2010).
[2] Liverpool, T. B. Phys. Rev. E 101(4), 042107 apr (2020).
[3] Jarzynski, C. Phys. Rev. Lett. 78(14), 2690–2693 apr (1997).
[4] Markowich, P. A. and Villani, C. Mat. Contemp. 19, 1–29 (2000).

P13

Augur Network Facilitates Protein Discovery and Design

Adam Kuhn[A] José Onuchic[A,B] Vinícius Contessoto[A,B]

Proteins Do Everything!

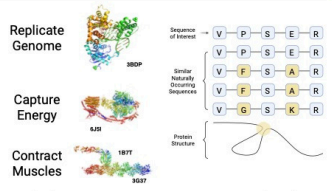


Fig 1. (Left) Proteins are functional heteropolymers. (Right) Direct coupling analysis (DCA)[1] can be used to calculate the 3D structure given a protein's 1D amino acid sequence. This connection between sequence, structure, and function has been used in neural networks like Evo2 and ESM.

Foundation Models Have Limited Generative Potential

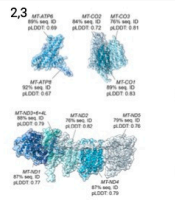


Fig 2. AlphaFold3[2] predicted structures for Evo2[3] generated proteins. Sequence similarity between natural and de novo proteins ranges from 76%-92%.

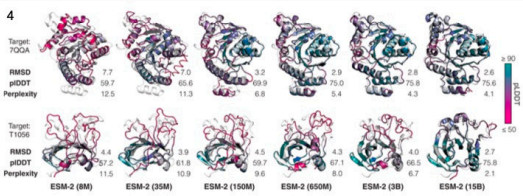


Fig 3. ESMFold[4] predicts protein structures from amino acid sequence. ESMFold learned 3D constraints implicitly during training and does not generate a multiple sequence alignment (MSA) at inference making it much faster than AlphaFold for structure prediction. This makes ESMFold an ideal candidate for evaluating the biophysical efficacy of large numbers of proposed de novo protein sequences.

Future Directions

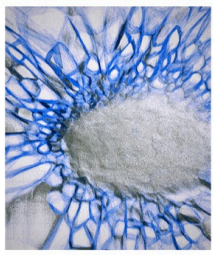
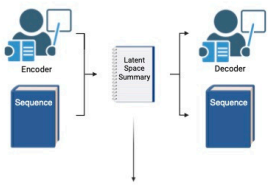


Fig 8. The Augur latent space can be compressed and visualized interactively. Blue regions have high sequence entropy.

1. Produce a more sophisticated Variational Auto Encoder that can handle greater sequence diversity
2. Train on multiple protein families
3. Enable unconstrained exploration of protein sequence space

Variational Autoencoders Learn Rich, Abstract Representations of Proteins



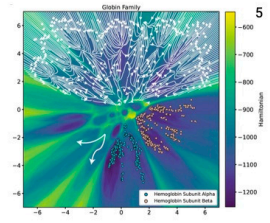


Fig 4. Variational autoencoders store information in a vector space called a latent space. A latent space can be sampled and each point annotated to generate an organized landscape of possible sequences.

Augur Generated SH3 Proteins are Novel and Biologically Plausible

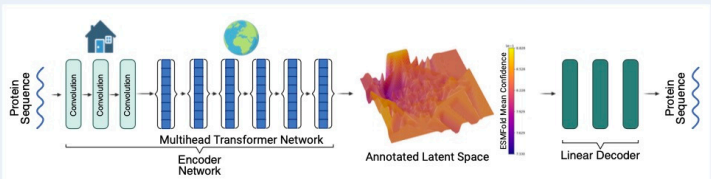


Fig 5. Augur is a variational autoencoder whose latent space is annotated by foundation models. Tokenized protein sequences are encoded through convolutions and a transformer network to capture both local and global sequence patterns. The decoder is simple to encourage latent organization.

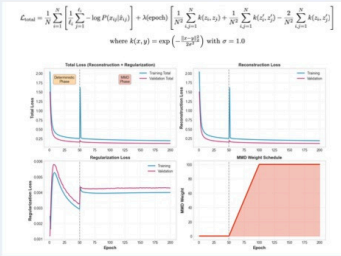


Fig 6. Augur is trained progressively. First it learns to reconstruct sequences from latent codes using an L2 penalty. Then it regularizes its latent space using a Maximum Mean Discrepancy (MMD) loss term.

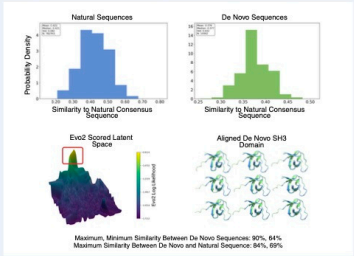


Fig 7. Augur generates sequences with comparable diversity to naturally occurring sequences. By sampling the latent space and scoring each sequence with Evo2 we can find sequences that fold naturally.

Conclusions

Augur learns rich representations of proteins.

Sampling Augur's latent space can produce new proteins with desired properties.

Foundation models such as Evo2 and ESMFold offer an unconstrained alternative for latent space functional annotation.

References

1. F. Morcos et al. Direct-coupling analysis of residue coevolution captures native contacts across many protein families, PNAS, 2011
2. Abramson, J., Adler *et al.* Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature, 2024*
3. Eric Nguyen et al. Sequence modeling and design from molecular to genome scale with Evo, Science, 2024
4. Zeming Lin et al. Evolutionary-scale prediction of atomic-level protein structure with a language model, Science, 2023
5. Ziegler, C. et al. Latent generative landscapes as maps of functional diversity in protein sequence space, Nature Communications, 2023

Acknowledgements

The authors would like to thank The Center Theoretical Biological Physics[A], Rice University Physics Department[B], and The National Science Foundation for their generous and persistent support for this work.

P14

SUPRA-LINEAR STORAGE IN DENSE NETWORKS OF GRID AND PLACE CELLS

Adriano Barra[1], **Martino S. Centonze**[2], **Michela Marra Solazzo**[3], **Daniele Tantari**[2]

[1]*Dipartimento di Scienze di Base ed Applicate per l'Ingegneria, Sapienza Università di Roma, Italy; INFN, Sezione di Roma1; CNR Nanotec, Salento Unit, Lecce, Italy.*
[2]*Dipartimento di Matematica, Università di Bologna, Italy.*
[3]*Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, Italy.*

Place cells are hippocampal neurons that activate in specific regions of the environment, forming the building blocks of internal spatial representations. Place-cell networks are commonly used to model cognitive maps, but their classical formulation relies on pairwise Hebbian synapses [1], which strongly limit storage capacity. In these models, the number of spatial maps that can be stored grows only linearly with network size, a regime that is not sufficient for realistic three-dimensional navigation. Representing two-dimensional surfaces embedded in 3D environments requires instead a supra-linear number of patterns.

Dense Hebbian architectures, where higher-order neural assemblies contribute to memory storage, offer a promising way to overcome this limitation. Recent work has shown that many-body generalizations of Hopfield-type networks remain biologically plausible while supporting high-capacity associative memory [2, 3]. Within this perspective, a simple two-layer architecture is examined: a layer of place cells and a second layer encoding internal spatial representations reminiscent of grid cells. When place cells are assumed to interact with pairs of grid-like units, the resulting model becomes equivalent to a dense Battaglia-Treves [4] network endowed with effective four-body interactions.

Using analytical methods from the statistical mechanics of disordered systems – in particular Guerra's interpolation under replica symmetry – it is possible to derive the self-consistency equations and compute the full phase diagram. The analysis shows that higher-order neural assemblies can sustain a supra-linear number of continuous attractors, providing a biologically grounded mechanism for high-capacity spatial memory. Numerical simulations further illustrate the robustness of the architecture in supporting recognition and navigation on general surfaces embedded in three-dimensional space [5].

Overall, this framework highlights the computational advantages of dense coding in hippocampal circuits and offers a theoretical route toward understanding large-capacity cognitive maps in realistic environments.

This work is inspired by a recent joint collaboration on dense spatial representations and continuous attractors [5], developed together with A. Barra, M. S. Centonze and D. Tantari.

[1] M. S. Centonze, A. Treves, E. Agliari, A. Barra, J. Stat. Phys. 192, 1 (2025).
[2] D. Krotov, J. J. Hopfield, arXiv:2008.06996 (2020).
[3] E. Agliari, L. Albanese, F. Alemanno, A. Alessandrelli, A. Barra, F. Giannotti, D. Lotito, D. Pedreschi, Physica A 626, 129076 (2023).
[4] F. P. Battaglia, A. Treves, Phys. Rev. E 58, 7738 (1998).
[5] A. Barra, M. S. Centonze, M. M. Solazzo, D. Tantari, arXiv:2511.02441 (2025).

P15

Resource-mediated interactions shape spatial patterns in individual-based models of vegetation dynamics

Vinicius M. Muccillo[1], **Ricardo Martínez-García**[2,1,3]

[1] *Instituto de Física Teórica, Universidade Estadual Paulista - UNESP, Brazil*
[2] *Center for Advanced Systems Understanding (CASUS) – Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Untermarkt 20, Görlitz 02826, Germany*
[3] *ICTP South American Institute for Fundamental Research*

Spatial pattern formation is a central phenomenon in ecology. In water-limited ecosystems, plants often arrange into spatial patterns, including gaps, labyrinths, and spots, as they compete for the little available water. These self-organized structures arise from the interplay between facilitative and competitive plant interactions, mediated by resource availability, acting at different spatial scales. Consequently, understanding how these patterns originate and persist under different environmental conditions requires models that link individual behaviour, resource dynamics, and spatial feedbacks in plant interactions.

Mathematical models describing this phenomenon belong mainly to two classes. The first class consists of individual-based models (IBMs), which represent each organism and its interactions explicitly in space. In most IBMs applied to vegetation, competition for limiting resources (particularly water) is incorporated implicitly: the resource itself does not appear as a state variable. Instead, demographic rates are modulated by local crowding, often through a kernel function that weights the influence of neighboring plants. Because they track individual organisms and stochastic events, IBMs quickly become computationally expensive, especially at large spatial scales or high densities. The second class consists of density-based models that describe the spatiotemporal dynamics of vegetation biomass density fields using partial differential equations. In contrast to IBMs, these models typically represent resources explicitly, introducing additional fields such as soil or surface water to capture consumer–resource dynamics. Density-based models are computationally less expensive and mathematically more tractable due to their formulation in terms of continuous PDEs.

I will present a hybrid approach to study vegetation pattern formation in water-limited ecosystems. This new model combines an individual-based representation of the plant population with a continuous, density-based description of water dynamics. Modeling water concentration explicitly allows us to understand more clearly how the spatial feedbacks between resource availability and local demographic processes generate and maintain different vegetation patterns, with plant interactions emerging indirectly through shared access to water rather than being imposed via a kernel function. At the same time, representing plants at the individual level preserves important biological detail by maintaining explicit demographic stochasticity, life-cycle stages, and localized dispersal. I will present a preliminary analysis of this model, mainly based on intensive numerical simulations and analytical approximations, demonstrating how spatial feedbacks between plant density and resource redistribution control the emergence, stability, and geometry of vegetation patterns.

P16

Interplay of Hexatic Order and Hyperuniformity in Model Biological Tissues

Mostafa Alkady[1], **Yiwen Tang**[1], **and Dapeng Bi**[1]

[1]*Department of Physics, Northeastern University*

Hyperuniformity and hexatic order represent two distinct forms of organization in many-body systems, characterized respectively by suppressed long-wavelength density fluctuations and quasi-long-range bond-orientational order. Both phenomena have recently been observed in models of confluent biological tissues [1,2], where collective cell dynamics can drive transitions between solidlike and fluidlike states. We explore the relationship between hyperuniformity and hexatic order in such active tissue systems, and whether the same mechanisms that control topological defect dynamics and orientational order might also regulate density fluctuations and hyperuniformity.

[1] Y. Tang, S. Chen, M. J. Bowick, D. Bi, Phys. Rev. Lett. 132, 218402 (2024).
[2] Y. Tang, X. Li, D. Bi, arXiv:2408.08976 (2024).

P17

Entropic Analysis of Cardiac Signals

Amanda Mollineda Rodríguez[1], **Ernesto Estévez Rams**[1,2]

[1] *Faculty of Physics*

[2] *Faculty of Physics - Institute of Materials Science and Technology (IMRE), University of Havana*

Cardiovascular diseases are the leading cause of mortality worldwide. Among them, cardiac arrhythmias have a significant impact on public health, with atrial fibrillation (AFIB) being the most common and dangerous [1]. In this context, early detection and continuous monitoring of atrial fibrillation are essential for implementing timely and effective therapeutic strategies. This research develops a novel methodology to characterize atrial dynamics using entropic measures derived from information theory [2].

First, we analyzed multiple electrocardiographic (ECG) leads using distance matrices to visualize and quantify complex dynamic patterns. From these, we computed core entropic measures as quantitative descriptors of signal complexity and we trained a neural network to classify healthy individuals and atrial fibrillation patients, using only these entropic features as input. The entropy density (h), introduced as the primary descriptor, proved highly effective in capturing subtle, nonlinear physiological dynamics. We achieved a classification accuracy of 82.72% using two ECG leads (II and V1) from 10-second recordings — a reduction in data requirements compared to conventional methods, which typically rely on multiple leads or prolonged recordings. This efficiency, without sacrificing diagnostic performance, opens new pathways for low-cost, portable, and scalable cardiac monitoring systems.

Additionally, we performed an entropic characterization of bidimensional trajectories defined for the ECGs, with the aim of studying whether the geometry and dynamics of these trajectories contain information about the underlying processes of the cardiac conduction system. The entropic measures revealed an intrinsically more complex and heterogeneous dynamics in AFIB, manifested by multimodal and asymmetric distributions, consistent with the pathology.

Finally, we implemented and optimized Echo State Networks (ESN) for the prediction of cardiac behavior [3], obtaining promising results, particularly in forecasting stationary dynamics of both sinus rhythm and atrial fibrillation. The ability demonstrated by the ESN to capture quasi-periodic dynamics with subtle variations validates their potential to handle both the deterministic and stochastic characteristics inherent to the cardiovascular system.

[1] S. Bordignon, M.C. Corti, and C. Bilato. Atrial fibrillation associated with heart failure, stroke and mortality. Journal of Atrial Fibrillation, 5(1):12-39, 2012.

[2] T.M. Cover and J.A. Thomas. Elements of Information Theory. Wiley, 2006.

[3] J. Herbert. The echo state approach to analysing and training recurrent neural networks-with an erratum note. Bonn, Germany: German National Research Center for Information Technology GMD Technical Report, 148(34):13, 2001.

The Effect of Flocking on the Orientation of Migratory Species

F.Payandeh [1] , N.Berenjkar [1] , and M.D.Niry [1]

[1]Institute for Advanced Studies in Basic Sciences, Zanjan, Iran.

The problem accurate orientation and routing during migration is an important topic in both biology and the physics of complex systems. Experimental evidence shows that many migratory animals can reduce individual navigation errors and discover more optimal routes by flocking. In this thesis, using the Vicsek model and its extended version, we investigate the effect of flocking on orientation accuracy. In the basic model, each agent (BOID) determines its direction of motion based on the average orientation of its neighbors. In the extended version, a preferred direction component with added random noise is added to achieve a more realistic simulation of targeted orientation. Numerical results indicate that flocking, in the presence of noise, plays an important role in improving the alignment with the target direction and can shift the location of the turning point of the order parameter. Analysis of the angular variance between the BOIDs and the target also shows that flocking, especially under noisy conditions, can enhance orientation.

P19

Investigating chimera states in dynamical networks with adaptive coupling

Mohammad Nasir Rafat [1], **Mina Zarei** [2]

Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran

Many complex systems, such as the brain network, the internet, and social networks, can be modeled as a network. One of the fundamental issues in complex networks is investigating the mutual interaction between structure and dynamics; just as structure influences dynamics, dynamics can also influence structure. This phenomenon is studied under the title of adaptive networks. In the system examined in this research, the main components are neurons. Each neuron can respond to external stimulation in various ways, and this behavior can be modeled with a phase response curve. This curve shows how much an input stimulus advances or delays the phase of the neuron at which point in its oscillation cycle; in other words, it describes how it reacts to external stimulation. In addition, we can model changes in the coupling strength of neurons by applying Hebbian dynamics, anti-Hebbian dynamics, and synaptic plasticity. Within this general framework, it is observed that by changing the coupling strength and the type of phase response curve in different neurons, various dynamical structures such as two-cluster states, coherent state, chaotic state, chimera state and multilayer structure are formed. Subsequently, to make the network more realistic, we assume that 80% of the neurons are excitatory and 20% are inhibitory and proceed with the investigation.

[1] H. Sayama, Introduction to the Modeling and Analysis of Complex Systems (Open SUNY Textbooks, 2015).
[2] G. H. J. Lanel and H. S. S. P. Jayawardena, Int. J. Sci. Res. Publ. **10**, 9929 (2020).
[3] M. E. J. Newman, Proc. Natl. Acad. Sci. U.S.A. **103**, 8577 (2006).
[4] M. E. J. Newman, Europhys. Lett. **103**, 28003 (2013).
[5] S. Fortunato and D. Hric, Phys. Rep. **659**, 1 (2016).
[6] E. Ravasz and A.-L. Barabási, Phys. Rev. E **67**, 026112 (2003).
[7] T. Gross and H. Sayama, Adaptive Networks: Theory, Models and Applications (Springer, 2009), pp. 1–8.
[8] F. A. Rodrigues, T. K. D. M. Peron, P. Ji, and J. Kurths, Phys. Rep. **610**, 1 (2016).
[9] Z. Heyvaert, Ph.D. Thesis, Ghent University (2018).
[10] I. H. de Mendoza, L. A. Pachón, J. Gómez-Gardenes, and D. Zueco, Phys. Rev. E **90**, 052904 (2014).
[11] F. Dörfler and F. Bullo, SIAM J. Appl. Dyn. Syst. **10**, 1070 (2011).
[12] S. H. Strogatz, Nature **410**, 268 (2001).
[13] M. E. J. Newman, SIAM Rev. **45**, 167 (2003).
[14] G.-Q. Bi and M.-M. Poo, J. Neurosci. **18**, 10464 (1998).
[15] H. Markram, J. Lübke, M. Frotscher, and B. Sakmann, Science **275**, 213 (1997).
[16] S. H. Strogatz, Physica D **143**, 1 (2000).
[17] Y. Kuramoto, Chemical Oscillations, Waves, and Turbulence (Courier Corporation, 2003).
[18] E. M. Izhikevich, Phys. Rev. E **58**, 905 (1998).
[19] R. G. M. Morris, Brain Res. Bull. **50**, 437 (1999).
[20] T. Aoki and T. Aoyagi, Phys. Rev. E **84**, 066109 (2011).

P20

Logical model for intracellular signaling in CD8$^+$ T cells mediated by cytokines modulating the immune response

Lorena Ramos[1], **Karina García-Martínez**[2], **José A. Sánchez**[3], **Denis Thieffry**[4], and **Kalet León**[2]

[1]Faculty of Physics, University of Havana, Cuba
[2]Center for Molecular Immunology (CIM), Havana, Cuba
[3]Institut de Mathématique de Marseille, France
[4]École Normale Supérieure, Paris, France

November 2025

Abstract

The differentiation of CD8$^+$ T cells into effector or memory phenotypes is governed by a highly nonlinear and stochastic intracellular network, in which interleukin-2 (IL-2) and its variants (muteins NA and NASB) play a central role. This work develops and implements a logical model of intracellular signaling based on binary and multilevel nodes representing receptors, kinases, transcription factors, and metabolic pathways. The model was constructed in *GINsim* and analyzed through stochastic simulations using the *CoLoMoTo* and *MaBoSS* platforms.

Through the study of attractors, reachability analysis, and the computation of state and transition entropies, functional multistability is revealed: identical combinations of stimuli (e.g., IL-2 plus antigen presentation by APCs) can lead to distinct cellular fates with non-trivial probabilities. The analysis also highlights the critical roles of regulators such as STAT5, FOXO, SATB1, and mTOR in controlling the effector versus memory commitment. Furthermore, the muteins NA and NASB are shown to bias the signaling dynamics toward memory and effector states, respectively.

These results provide a formal platform for quantifying the plasticity and control points of CD8$^+$ T cell differentiation, offering insights relevant for the rational design of immunotherapies that modulate IL-2–mediated signaling.

Keywords: CD8$^+$ T cells; IL-2; NA and NASB muteins; logical modeling; GINsim; MaBoSS; CoLoMoTo; multistability.

References

1. Stoll, G., Rougemont, J., & Thieffry, D. (2012). Continuous time Boolean modeling for biological signaling: application of Gillespie algorithm. *BMC Systems Biology*, 6:116.
2. García-Martínez, K. (2018). Modelación matemática del papel de la IL-2 en la dinámica de las células T: estudio del efecto de tratamientos moduladores de la IL-2. *Frontiers in Immunology*, 9, 2987.
3. Naldi, A., Carneiro, J., Chaouiya, C., & Thieffry, D. (2010). Diversity and plasticity of Th cell types predicted from regulatory network modelling. *PLoS Computational Biology*, 6(9).

P21

Information Flow and Fractional Diffusion in Networks

Camilo A. Rozo[1], **Alejandro P. Riascos**[1]

[1]*National University of Colombia, Faculty of Science*

Understanding how information propagates across complex networks is essential for characterizing the multiscale organization that emerges from their topology. In this work, we develop a theoretical and computational framework to describe information flow in networks through the spectral properties of the graph Laplacian $\mathcal{L}$ [1]. Using the propagator $e^{-\tau\mathcal{L}}$, we define a density operator that captures the distribution of accessible diffusion states, allowing us to compute the von Neumann entropy and a heat-capacity-like quantity that identifies phase-transition-like regimes during the diffusion process [2]. These quantities reveal whether a network exhibits homogeneous or heterogeneous multiscale propagation.

We apply this formalism to classical ensembles such as Erdős-Rényi, Watts-Strogatz, and Barabási-Albert networks, as well as community-structured and real transportation networks. The results show that homogeneous ensembles display a single entropic transition, while networks with small-world structure or modular organization exhibit a hierarchy of nested transitions that reflect their mesoscale architecture.

We further introduce the fractional Laplacian $\mathcal{L}^{\gamma}$, with $0 < \gamma < 1$, which models long-range interactions [3]. Simulations on Watts-Strogatz networks show that decreasing the fractional exponent gradually suppresses the multiscale complexity characteristic of low rewiring probability, producing a more homogeneous diffusion regime and a fractional information core.

This framework provides new tools to characterize the structural and dynamical complexity of networks, highlighting how diffusion processes encode the transition from segregated to integrated information across scales.

[1] De Domenico, M. Biamonte, J. (2016). Spectral entropies as information-theoretic tools for complex network comparison. Physical Review X, 6(4):041062.

[2] Villegas, P., Gabrielli, A., Santucci, F., Caldarelli, G. Gili, T. (2022). Laplacian paths in complex networks: Information core emerges from entropic transitions. Physical Review Research, 4(3):033196.

[3] Riascos, A. P. Mateos, J. L. (2021). Fractional Dynamics on Networks and Lattices. Springer Series in Complexity.

P22

An Adaptive Q-Learning Controller for Microrobots in Dynamic Thermal Environments

Aminreza SafarpourDobakhshary[1], **S.M.Sadegh Movahed**[1,2]

[1]*Department of Physics, Shahid Beheshti University, G.C., Evin, Tehran 19839, Iran*
[2] *School of Physics, Institute for Researches in Fundamental Sciences, P.O. Box 193955531, Tehran, Iran*

This research focuses on the design and implementation of an intelligent control system based on reinforcement learning for guiding particles in complex and dynamic environments. The project employs a specialized pathfinding microrobot trained using the Q-learning algorithm. The developed simulation incorporates environmental temperature as a vital and dynamic parameter that directly influences factors such as particle diffusion rates and robot performance. This precise modeling enables the simulation of real-world conditions, allowing the system to operate optimally in complex environments. Among the main challenges of this research is the design of an effective reward mechanism that accounts for thermal variations. This mechanism must be capable of providing optimal pathfinding to reach a specified target. This advanced system will be able to track a target in the shortest possible time and select the most efficient path by analyzing environmental parameters. The most significant applications of this technology include infiltrating tumor tissues and targeted drug delivery, which operate completely autonomously without the need for external control. Furthermore, the applications of this technology in various medical fields, particularly in targeted cancer therapies, are highly promising and could bring about a significant transformation in the field of medical technologies. By leveraging the latest advancements in artificial intelligence, this system offers a novel approach to precision medicine.

[1] Monderkamp, Paul A., et al. "Active particles using reinforcement learning to navigate in complex motility landscapes." Machine Learning: Science and Technology 3.4 (2022): 045024.
[2] Kaur, Harpreet, Thomas Franosch, and Michele Caraglio. "Adaptive active Brownian particles searching for targets of unknown positions." Machine Learning: Science and Technology 4.3 (2023): 035008.

P23

Viability of Transition Metal-Doped Tin Nanotechnology as Biosensor Material for Neural Disorder Detection

Nowshin Tabassum Riya [1], Noor Ahammad[1], Aoly Ur Rahman [2,3], Md. Alamgir Kabir[1] and Md. Kabir Uddin Sikder[1]

[1]Department of Physics, Jahangirnagar University, Savar, Dhaka, Bangladesh
[2]Department of Nanomaterials and Ceramic Engineering, Bangladesh University of Engineering & Technology, Dhaka, Bangladesh
[3]Department of Physics, Dhaka University of Engineering & Technology, Gazipur, Bangladesh

Gamma-aminobutyric acid (GABA) is the foremost inhibitory neurotransmitter of mammals' central nervous systems (CNS) responsible for different cognitive and behavioral functions such as insomnia, epilepsy, seizures, depression, anxiety, alcoholism, and premenstrual syndrome [1]. Therefore, for proper health management, a facile, rapid, and non-invasive method of monitoring GABA levels is crucial. However, in the era of nanotechnology, nanoclusters have drawn the attention of scientists due to their higher sensitivities, chemical stabilities, surface-to-volume ratio, recommendable electrochemical and optical tunability, etc. making them potentially useful in different biomedical applications, especially in high-performance sensing devices [2]. Among various nanoclusters, tin has a comprehensive oxidation state and a semiconducting nature, causing their higher chemical stabilities, sensitivity, and selectivity, making them prominent in developing different biosensors [3]. This work proposes a theoretical investigation of detecting GABA with transition metals (Cr, Mo, W) doped small tin nanocluster (Sn_6) by employing the quantum mechanical density functional theory (DFT) approach. From the analysis, it has been found that the Sn_5Cr nanocluster has a decreased adsorption length, whereas the adsorption mechanism increases energy significantly (around 21.6%) making it promising for developing biosensors for GABA detection. In addition, the IR Spectrum reveals no imaginary frequency which confirms the formation of complex adsorbate adsorbent systems to the lowest energy minima as well as the highest structural stability [4]. Moreover, the study of other electrical and optical properties of the complex discloses its possibility of being useful in sensory devices for GABA detection.

[1] L. D. Ochoa-de la Paz *et al.*, "The role of GABA neurotransmitter in the human central nervous system, physiology, and pathophysiology," *Rev. Mex. Neurocienc.*, vol. 22, no. 2, pp. 67–76, Apr. 2021, doi: 10.24875/rmn.20000050.

[2] H. Nasrollahpour, B. J. Sánchez, M. Sillanpää, and R. Moradi, "Metal Nanoclusters in Point-of-Care Sensing and Biosensing Applications," *ACS Appl. Nano Mater.*, vol. 6, no. 14, pp. 12609–12672, Jul. 2023, doi: 10.1021/acsanm.3c01569.

[3] B. Peters, N. Lichtenberger, E. Dornsiepen, and S. Dehnen, "Current advances in tin cluster chemistry," *Chem. Sci.*, vol. 11, no. 1, pp. 16–26, 2020, doi: 10.1039/C9SC04363B.

[4] A. Ur Rahman, D. Mohammad Saaduzzaman, S. Mahedi Hasan, and Md. Kabir Uddin Sikder, "A DFT Investigation on Structural, Electric, and Thermodynamic Properties of Transition Metal (Cr, Mo, and W) Doped in Small Arsenic Cluster (As15)," in *2022 4th International Conference on Sustainable Technologies for Industry 4.0 (STI)*, Dec. 2022, pp. 1–6. doi: 10.1109/STI56238.2022.10103244.

P24

CrystalGRW: Generative Modeling of Crystal Structures with Targeted Properties via Geodesic Random Walks

Krit Tangsongcharoen,[1,2,*] Teerachote Pakornchote,[3,†] Chayanon Atthapak,[1] Natthaphon Choomphon-anomakhun,[1] Annop Ektarawong,[1,4] Björn Alling,[5] Christopher Sutton,[3] Thiti Bovornratanaraks,[1,2,‡] and Thiparat Chotibut[4,§]

[1] *Extreme Conditions Physics Research Laboratory and Center of Excellence in Physics of Energy Materials (CE:PEM), Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

[2] *Thailand Center of Excellence in Physics, Ministry of Higher Education, Science, Research and Innovation, 328 Si Ayutthaya Road, Bangkok 10400, Thailand*

[3] *Department of Chemistry and Biochemistry, University of South Carolina, South Carolina 29208, USA*

[4] *Chula Intelligent and Complex Systems Lab, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

[5] *Theoretical Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, SE-581 83 Sweden*

(Dated: July 27, 2025)

Determining whether a candidate crystalline material is thermodynamically stable depends on identifying its true ground-state structure, a central challenge in computational materials science. We introduce CrystalGRW, a diffusion-based generative model on Riemannian manifolds that proposes candidate crystal configurations in stable phases, validated through density functional theory calculations. The crystal properties, such as fractional coordinates, atomic types, and lattice matrices, are represented on suitable Riemannian manifolds, ensuring that new predictions generated through the diffusion process preserve the periodicity of crystal structures. We incorporate an equivariant graph neural network to also account for rotational and translational symmetries during the generation process. CrystalGRW demonstrates the ability to generate realistic crystal structures that are stable and closely resemble their density functional theory ground states. It also enables conditional control, such as specifying a desired crystallographic point group, which helps accelerate materials discovery and inverse design by offering stable, symmetry-consistent crystal candidates for experimental validation.

I. INTRODUCTION

Crystal structures, defined as the periodic arrangement of atoms in a lattice, directly influence material properties such as stability, band gap, and mechanical strength. Understanding and predicting the behavior of materials from the atomistic level relies on knowing accurate structures. The search for novel materials involves identifying crystal structures and their compositions that are thermodynamically metastable. However, this task is complicated by the vast number of degrees of freedom that must be explored to identify local minima on the free energy surface [1, 2].

Many advanced algorithms for sampling configurations on the potential energy surface have been developed for ground state structure prediction, these approaches typically combine (stochastic) samples technique such as evolutionary algorithms, *ab-initio* random structure searching, simulated annealing, metadynamics, basin hopping, and molecular dynamics simulations [2–8], with quantum mechanics-based method, such as density functional theory (DFT) to accurately predict the energy of the sampled configurations. However, the cubic scaling with respect to the number of basis functions in DFT leads to a substantial computational time for searching for new candidate materials. Machine-learned interatomic potentials (MLIPs) are an accurate and efficient alternative to DFT [9–17], and therefore can speed up the prediction process. Nonetheless, improving the structure generation task remains an important challenge for materials discovery.

Instead of the traditional approach of starting from an initial structure and performing sampling to find new (possibly lower energy) structures, generative models enable a direct and much more efficient way to produce novel molecular and crystal structures because they can sample new materials given knowledge from the learned data distribution without being constrained by energy barriers [18–28]. Diffusion-based generative models draw principles from non-equilibrium thermodynamics to transform random noise into structured data [29–32]. These models generate samples through stochastic differential equations (SDEs) that consist of data-dependent drift and diffusion terms. The Brownian motion component introduces stochastic noise, enabling the generation of new crystal structures [30]. Recent works show that properly designed diffusion models can generate crystal structures with realistic characteristics, such as atoms do not overlap, lattice parameters are rea-

* These authors contributed equally to this work.
† These authors contributed equally to this work.; Correspondence to: pakornct@mailbox.sc.edu
‡ Correspondence to: thiti.b@chula.ac.th
§ Email: thiparatc@gmail.com

P25

Abstract template for Spring College in the Physics of Complex Systems 2026 The Architecture of Cortical Timing: From Local Clustering to Global Hierarchies

Sara Varetti[1], **Merav Stern**[2]

[1]*International School for Advanced Studies (SISSA)*
[2]*Rockefeller University*

Cortical circuits exhibit spontaneous activity characterized by a hierarchy of timescales that reflects the anatomical hierarchy of cortical regions [1]. Such long-ranging intrinsic dynamics, which extend beyond the duration of typical sensory stimuli, are thought to facilitate the integration of information over multiple temporal scales. Stern et al. [2, 3] have shown that clustered network architectures can intrinsically generate heterogeneous timescales and support long temporal fluctuations when the local clustering of neurons is substantial. We propose that variations in clustering strength across cortical areas contribute to the observed hierarchy of intrinsic timescales. To test this, we model a feedforward chain of neural networks, each representing a local circuitry, endowed with neural assemblies (clusters) whose activity follows $\frac{dx_i^{(d)}}{dt} = -x_i^{(d)} + s_d\phi(x_i^{(d)}) + \sum_{j=1}^{N_d} J_{ij}^{(d)}\phi(x_j^{(d)}) + \sum_{j=1}^{N_{d-1}} W_{ij}^{(d)}\phi(x_j^{(d-1)})$. Within each local network, the clustering affects the autocorrelation of the local population activity, generating local timescales that are also transmitted downstream as temporally correlated (colored) input noise. We examine how the intra-areal structured activity is propagated and interacts with the downstream population, and under which conditions these interactions can give rise to a gradient of intrinsic timescales across the chain. Our analysis reveals that a hierarchy of intra-clustering strengths, corresponding to increased clustering in strength and size, is essential to reproduce the cortical gradient of intrinsic timescales. In contrast, stronger feedforward coupling reduces the diversity of timescales. In the Dynamic Mean-Field description, the effective input to area d has covariance $\langle \eta_d(t)\eta_d(t')\rangle = g_d^2\, C_{\phi^d}(t,t') + f_d^2\, C_{\phi^{(d-1)}}(t,t')$, showing that feedforward input acts as an additional colored perturbation inherited from the upstream network. To analyze how this temporally correlated input reshapes the downstream dynamics, we used the unified colored noise approximation. Assuming $\tau_{d-1} \leq \tau_d$ and $f_d \propto g_d$ leads to an impact shift of $\log\langle\tau_d\rangle \propto \frac{\tau_{d-1}}{D_{eff}^{(d-1)}}$ with $D_{eff}^{(d-1)} = f_d^2 \int C_{\tilde{\eta}_d}(\tau)d\tau$ the color noise strength. Hence, increasing the feedforward coupling f reduces the subsequent network timescale. Finally, analyses of neuronal activity recordings show that deeper cortical layers display stronger functional clustering and longer intrinsic timescales, consistent with our model's predictions. Together, these results provide a framework linking local recurrent architecture with inter-areal connectivity to the emergence of hierarchical cortical timescales, offering insight into how transient stimuli are integrated and transformed into long neural trajectories needed for cognitive functions.

[1] J. D. Murray, A. Bernacchia, N. A. Roy, A. Constantinidis, R. Romo, X.-J. Wang, Nat. Neurosci. **17**, 1661 (2014).
[2] M. Stern, H. Sompolinsky, L. F. Abbott, Phys. Rev. E **90**, 062710 (2014).
[3] M. Stern, N. Istrate, L. Mazzucato, eLife **10**, e65421 (2021).

P26

Self-Control of Supertransient Collective Chaos in Coupled Map Networks

Jhon S. Villacís Ramón[1], **Mario G. Cosenza Miceli**[1]

[1]*School of Physical Sciences and Nanotechnology, Yachay Tech University, Urcuquí 100119, Ecuador*

Supertransient collective chaos is an emergent phenomenon that consists of the appearance of a chaotic time window (before reaching a stable state) when periodic elements are locally coupled together, with the particularity that the length of this chaotic window depends exponentially on the number of coupled elements. Thus, being a nontrivial and unexpected phenomenon in which collective chaos arises from local stable periodic elements. In this work, we study how various system parameters, including the network topology, affect the length of the chaotic window. We propose a mechanism for autonomous control of this phenomenon. Our method can be extended to networks of coupled time-continuous periodic dynamical systems.

P27

Modeling Language Evolution Using a Spin Glass Approach

Hediye Yarahmadi*[1], Alessandro Treves[1]

[1]*Cognitive Neuroscience, SISSA, Trieste, Italy*

1. Introduction

Recent advances in phylogenetic linguistics by Longobardi and colleagues [1], based on syntactic parameters, seem to reconstruct language evolution farther in the past than traditional etymological approaches. Combined with quantitative statistics, this Parametric Comparison Method also raises general questions: why does syntax keep changing? Why do languages diversify instead of converging into efficient forms? And why is this change so slow, over centuries? We hypothesize that the fundamental reasons are disorder and frustration: syntactic parameters interact through disordered interactions, subject to weak external drives and, unable to settle into a state fully compatible with all interactions, they evolve slowly with "glassy" dynamics.

2. Model

To explore such hypothesis, we model a "language" as a binary vector of the 94 syntactic parameters considered in the Longobardi database, and assume that they interact both through the explicit and asymmetric dependencies that linguists call "implications" (which may lead to rotating changes [2]) and through weak, partly asymmetric interactions, which we assign at random an inverse relative strength ζ and a degree of asymmetry φ ranging from 0° (symmetric) to 90° (fully antisymmetric). Using Glauber dynamics, we simulate the evolution of these parameters, assuming external fields to only set the initial conditions.

3. Results

Fig. 1 sketches the (ζ,φ) phase diagram based on simulations of the average number of parameters flip in the asymptotic phase. Syntactic parameters get trapped in a steady state (one of a disordered multiplicity) for low asymmetry, while they continue to evolve for higher asymmetry. The strength of the random interactions is almost irrelevant, but when they dominate ($\zeta \to 0$), the transition is sharp at $\varphi = 30°$. For high ζ, dynamics is slow, but at ($\zeta \to \infty$), they continue indefinitely: implications alone allow no steady state.

4. Discussion

The sharp transition at $\varphi = 30°$ for $\zeta \to 0$ aligns with previous studies of asymmetric spin glasses [3] ($\eta = 1/2$ in their notation), indicating that varying the interaction symmetry induces a phase transition from glassy to chaotic dynamics. This suggests that to understand language evolution in the syntax domain it is essential to include, along the implicational structure constraining parameter changes, disordered interactions which have so far eluded linguistic analysis, in part because of their quantitative rather than logical nature.

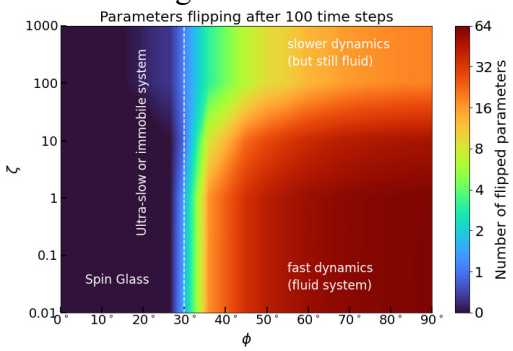


Fig. 1. Phase diagram ($\zeta - \varphi$): The system freezes with symmetric interactions (up to $\varphi \approx 30°$) and becomes fluid as asymmetry increases for small ζ. Similar behavior occurs to large ζ, but with slower fluid dynamics, and with $\zeta \to \infty$, it is chaotic.

[1] A. Ceolin, C. Guardiano, G. Longobardi et al., Phil. Trans. Roy. Soc. B 376(1824), 20200197 (2021).
[2] P. Crisma, G. Fabbris, G. Longobardi, C. Guardiano, J. Historical Syntax 9, 1–26 (2025).
[3] K. Nutzel, U. Krey, J. Phys. A: Math. Gen. 26, L591 (1993).

P28

SIMULATION OF FLUID DYNAMICS USING CFD, PHYSICS-INFORMED NEURAL NETWORKS, AND STOCHASTIC METHODS

Muhammad Zulqurnain[1]

[1]*Abdus Salam School of Mathematical Sciences (ASSMS), Government College University (GCU), Lahore, Pakistan*

This work presents a simulation-based framework for modeling incompressible fluid flows using both traditional and modern computational approaches. I perform numerical simulations of the Navier–Stokes equations using OpenFOAM's finite-volume solvers, analyzing velocity profiles, pressure fields, and convergence behavior for laminar flows. In parallel, I implement Physics-Informed Neural Networks (PINNs) as mesh-free simulators capable of learning fluid solutions directly from the governing PDEs. PINN simulations allow flexible geometries, automatic differentiation, and direct enforcement of physical laws in the loss function.

To capture uncertainties in system parameters, I incorporate stochastic simulation through Markov Chain Monte Carlo (MCMC), estimating viscosity, inflow conditions, and other parameters based on observed or synthetic data. This enables quantification of uncertainty in both CFD and PINN simulations and provides insight into solver robustness under imperfect or noisy inputs.

The goal of this study is to compare simulation accuracy, computational efficiency, and stability across CFD, PINNs, and stochastic approaches, contributing to scalable and hybrid simulation techniques for complex fluid systems.

[1] OpenFOAM Foundation, OpenFOAM User Guide.
[2] M. Raissi et al., J. Comput. Phys. **378**, 686 (2019).
[3] R. M. Neal, Bayesian Learning for Neural Networks, Springer (1996).