



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

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

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Self-Control of Supertransient Collective Chaos in Coupled Map Networks

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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  $\phi = 30^\circ$ . Results suggest that disorder critically shapes slow, long-term syntactic change.

P01

Stochastic Optimal Control of differential equations using the maximum principle.

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

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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  $L \rightarrow \infty$ . 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.

## Modeling Enzyme Network Structure via Centrality Correlations

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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

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

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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.

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# Quantifying Consensus in Effective Model Inference for Disordered Ising Systems

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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.

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

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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.

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P07

Versatile reservoir computing for  
heterogeneous complex networks

## Stemness Percolation in Tumorspheres

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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.

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

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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- $\beta$ -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- $\beta$ ; Alzheimer's disease

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## Chimera games emerging from coevolutionary dynamics with endogenous feedbacks

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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.

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## Fuel-Driven Active Brownian Particles with Time-Dependent Propulsion

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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.

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

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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.

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

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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.

## Interplay of Hexatic Order and Hyperuniformity in Model Biological Tissues

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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.

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## Entropic Analysis of Cardiac Signals

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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.

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## The Effect of Flocking on the Orientation of Migratory Species

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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.

## Investigating chimera states in dynamical networks with adaptive coupling

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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.

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# Logical model for intracellular signaling in CD8<sup>+</sup> T cells mediated by cytokines modulating the immune response

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## Abstract

The differentiation of CD8<sup>+</sup> 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<sup>+</sup> T cell differentiation, offering insights relevant for the rational design of immunotherapies that modulate IL-2-mediated signaling.

**Keywords:** CD8<sup>+</sup> T cells; IL-2; NA and NASB muteins; logical modeling; GINsim; MaBoSS; CoLoMoTo; multistability.

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## Information Flow and Fractional Diffusion in Networks

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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.

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

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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.

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

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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 ( $\text{Sn}_6$ ) by employing the quantum mechanical density functional theory (DFT) approach. From the analysis, it has been found that the  $\text{Sn}_5\text{Cr}$  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.

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

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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 the-

ory (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-

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## Self-Control of Supertransient Collective Chaos in Coupled Map Networks

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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.

# Modeling Language Evolution Using a Spin Glass Approach

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## 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  $\zeta$  and a degree of asymmetry  $\varphi$  ranging from  $0^\circ$  (symmetric) to  $90^\circ$  (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  $(\zeta, \varphi)$  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 ( $\zeta \rightarrow 0$ ), the transition is sharp at  $\varphi = 30^\circ$ . For high  $\zeta$ , dynamics is slow, but at ( $\zeta \rightarrow \infty$ ), they continue indefinitely: implications alone allow no steady state.

## 4. Discussion

The sharp transition at  $\varphi = 30^\circ$  for  $\zeta \rightarrow 0$  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.

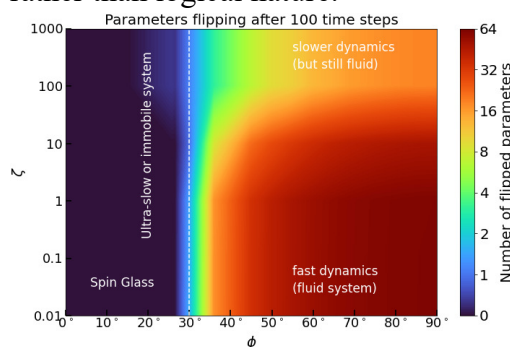


Fig. 1. Phase diagram  $(\zeta - \varphi)$ : The system freezes with symmetric interactions (up to  $\varphi \approx 30^\circ$ ) and becomes fluid as asymmetry increases for small  $\zeta$ . Similar behavior occurs to large  $\zeta$ , but with slower fluid dynamics, and with  $\zeta \rightarrow \infty$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

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