

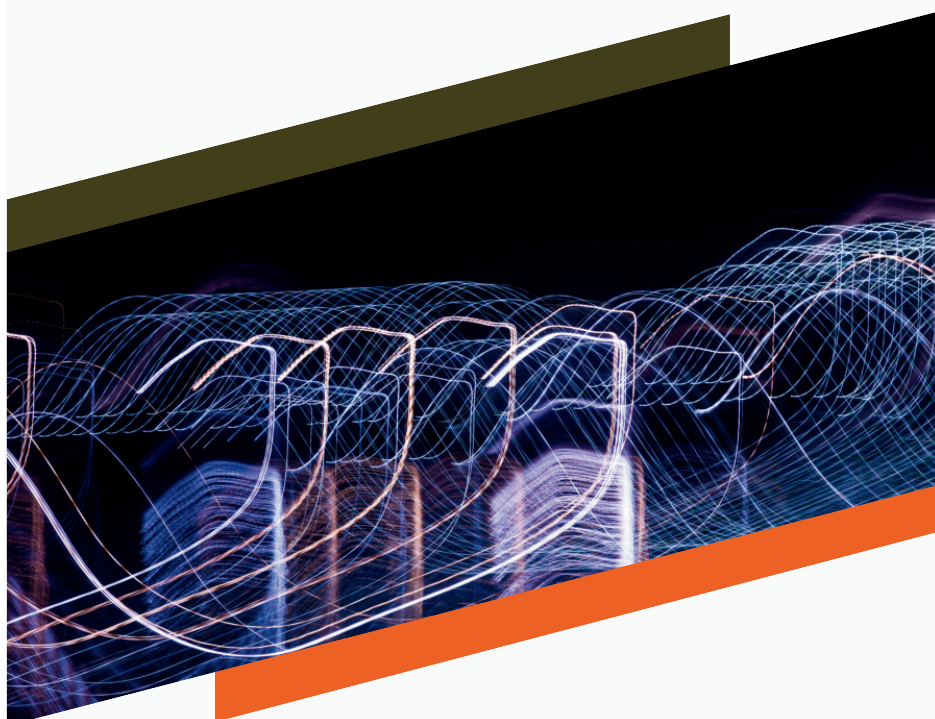


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Collective Phenomena in Disordered Systems- II



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Abstract For Talks

Waiting Times in Avalanche Processes: Universal Scaling and the Double Power-Law Hypothesis

Eduard Vives, Emma Valdés & Honglian Li, Department of Condensed Matter Physics, Physics Faculty, Universitat of Barcelona, Martí i Franquès, 1, 08028 Barcelona, Catalonia

Self-organized criticality (SOC) has long been recognized as a fundamental paradigm for understanding scale-invariant phenomena in complex systems, from fracture and avalanches to earthquakes. While the size distribution of events has been extensively studied, the temporal organization of these events remains less understood. In particular, the distribution of waiting times δ between avalanches provides key insights into the dynamics of energy release and the underlying critical state. In this work, we propose that waiting times in SOC systems follow a universal double power-law probability density function. This function is characterized by two critical exponents, α and β , which govern the scaling of short ($\sim \delta^{-\alpha}$) and long ($\sim \delta^{-\beta}$) waiting times, respectively, and by a crossover parameter δ_0 that sharply separates the two regimes. The parameter δ_0 , which depends on both system properties and observation conditions, acts as a scaling factor that collapses different distributions onto a single universal curve, consistent with Per Bak's original vision of universality in SOC [1]. To test this hypothesis [2], we analyze large labquake catalogs obtained from acoustic emission experiments during the uniaxial compression of porous charcoal samples with varying hardness. These experiments provide controlled conditions to explore the statistical properties of fracture avalanches. For labquakes, the fitted exponents consistently fall within $\alpha = 0.9 \pm 0.1$ and $\beta = 2.0 \pm 0.3$, with deviations attributable to sample-to-sample variability, suggesting that these values may be universal. We further compare these results with earthquake catalogs, where the observed exponents exhibit larger deviations, likely due to additional complexities such as spatial heterogeneity, finite-size effects, and catalog incompleteness.

References

1. Per Bak How Nature Works: The Science of Self Organized Criticality (Copernicus, New York 1996).
2. Honglian Li, Emma Valdés and Eduard Vives (2024), Double power law universal scaling function for the distribution of waiting times in labquake catalogues, Phys. Rev. E 110, 064140.

Nucleation and Propagation of Cracks in Fiber Bundle Model

Purusattam Ray, The Institute of Mathematical Sciences, Chennai, India

The nucleation and the subsequent growth of domains in various models have been studied thoroughly in equilibrium and non-equilibrium statistical mechanics. We discuss the nucleation

and propagation of cracks (domain of broken bonds) in fiber bundle model (FBM), a prototypical threshold activated dynamical system and a paradigm for studying material failure in physics and engineering. We discuss the origin of two length scales associated with the crack length and modified Griffith's law observed in experiments. We discuss the role of disorder and fracture process zone in the context of breaking dynamics in FBM.

Failure mechanics of Aneurysmatic Tissues

Anshul Faye, Department of Mechanical Engineering, Indian Institute of Technology Bhilai,
India

Abdominal aortic aneurysm (AAA) rupture is one of the prominent causes of death, particularly among elder persons, and it remains a major concern in vascular health. The mechanics of aneurysm ruptures are complicated and impacted by factors such as tissue anisotropy, calcification, micro-cavities, and collagen fiber alignment. Despite extensive research, predicting rupture remains challenging due to the non-linear, anisotropic characteristics of aneurysmatic tissue, which is exacerbated by the presence of calcification and cracks. This study looks at the mechanical behavior and failure processes of AAA tissue, including the role of tissue anisotropy, calcification, and microstructural defects in rupture initiation. A micromechanics-based numerical technique is used to simulate AAA tissue as a composite material, with the matrix representing the anisotropic tissue and calcium deposits represented as randomly distributed inclusions. With the help of finite element simulations the impact of biaxial loading, tissue stiffness, and collagen fiber orientation on rupture behavior is understood. The work brings out the impacts of crack orientation, loading direction in the presence of cracks. The findings suggest that calcification stiffens the tissue and makes it more isotropic, resulting in earlier failure at lower stretches, but collagen fibers play an important role in determining failure direction. Overall, the study emphasizes the role of defects such as calcification and cracks in influencing AAA tissue failure behavior, giving valuable insights for improved rupture prediction models.

Interfacial Slip in Elasto-Frictional Systems

Sohom Roy, Department of Earthquake Engineering, Indian Institute of Technology Roorkee

Interfacial slip is a pervasive phenomenon in nature, such as in glacier beds, landmasses' movements, crustal faults, and subduction zones, and it is a precursor to geological events such as catastrophic landslides and earthquakes. We investigate quasi-dynamic slip development on frictional interfaces within an elastically deformable bounding medium. We consider frictional strength to be slip rate- and state-dependent, which exhibits instantaneous strengthening in response to a sudden increase in slip velocity, followed by eventual weakening to a steady-state over a characteristic slip D_c . The difference in the magnitudes of instantaneous strengthening and subsequent weakening, in a homogenous interface, determines whether a perturbation to steady

quasistatic slip can diffuse aseismically in a nonlinear manner or diverge in finite-time. The interfacial slip rate diffusion are relevant to the accelerated creep of landmass and the finite-time instabilities in slip rate are relevant to dynamic rupture nucleation in catastrophic landslides. We further examine heterogeneities in frictional properties and explore how breaking translational symmetry results in slip complexity.

Emergent Glassy Dynamics in Active Tissues

Dipjyoti Das, IISER Kolkata, Kalyani, India

Collective cell movement drives crucial biological processes, including cancer invasion, wound healing, and embryo development. Yet, how tissue-scale material properties emerge from cellular interactions remains unclear. In this talk, I will introduce an active particle-spring model of tissue monolayers that captures the transition from a fluid-like to a solid-like state with increasing cell-cell adhesion, as reported in experiments. Close to the liquid–solid transition, the system exhibits glassy dynamics marked by subdiffusive motion, swirling velocity fields, and non-Gaussian displacement statistics, indicating a dynamically heterogeneous tissue. By eliminating many ad hoc assumptions of previous frameworks, our model offers a unified and minimal description of tissue mechanics, with broad implications for understanding collective cell behaviors in development, physiology, and disease.

Disorder-Induced Softening of Transitions in Multi-State Spin Systems

Manoj Kumar, National Institute of Science Education and Research, Bhubaneswar, India

In this work, we investigate the three-dimensional random-field Potts model (RFPM), focusing on its phase transition behavior, which is governed by a random fixed point located at zero temperature. Although determining ground states in the RFPM is an NP-hard problem, we employ a recently developed quasi-exact graph-cut-based scheme that enables efficient computation of ground states and systematic analysis of the critical behavior. Using this approach, we evaluate several key observables, such as magnetization, Binder and energy cumulants, specific heat, and susceptibilities, and extrapolate them to the quasi-exact ground-state limit. These quantities are computed for a range of system sizes, allowing for an extensive finite-size scaling analysis to locate the critical point and characterize the magnetic ordering transition. Our results provide compelling evidence for a continuous disorder-induced transition, in contrast to the first-order transition observed in the pure system. Furthermore, the extracted critical exponents differ from those of both the three-state RFPM and the random-field Ising model (RFIM), indicating the emergence of a distinct universality class for the multi-state RFPM.

Damage propagation in a cold gas: hydrodynamics, core scaling and universality

R. Rajesh, The Institute of Mathematical Sciences, Chennai, India

Consider the perturbation of a cold gas by input of energy, either instantaneous or continuously. The resulting shock propagates through the gas in a self-similar manner. I will review the recent interest and work on this problem and discuss in detail the case of uniformly driven gases.

Glassy dynamics and devitrification of amphiphilic colloids adsorbed at an air-water interface

Ranjini Bandyopadhyay, Raman Research Institute, Bangalore, India

Surface-active colloids (e.g. soft PNIPAM microgels) adsorb at the air-water interface of a drying droplet. Using bright-field microscopy experiments and molecular dynamics simulations, we show that soft PNIPAM colloids at an air-water interface exhibit dynamic heterogeneity and structural disorder, signatures that are typically associated with glassy dynamics. Interestingly, we even observe a devitrification of these amorphous structures both in experiments and in molecular dynamics simulations.

Quantum Walk : Impact of Coin and Path disturbances

Sanchari Goswami, Vidyasagar College, Kolkata, West Bengal, India

Quantum walks have been studied rigorously for the last three decades and it has been found that quantum walks are quadratically faster compared to the Classical Random Walk. In this work, we study the effect of slight perturbation to the quantum coin. The motivation comes entirely from the experimental fact that the coin flip is realized with quarter and half wave plates which may introduce error in the rotation sometimes. For introduction of decoherence in form of perturbation to the coin the quantum to classical transition is studied. The mean square displacement, persistence and first passage for the walk are discussed for the walk. The second part of the study involves the effect of a moving detector on a discrete one dimensional Quantum Walk where the movement in the form of hopping/shifts. This is again extremely important in connection to experimental studies of quantum walk as there is always a detector involved. The occupation probability of sites in all the above cases can be estimated. This can be compared to that of an Infinite Walk. Typical scaling behaviors for several quantities can be observed in the above cases. The limiting behaviors of the walk can be compared to Infinite Walk, Semi Infinite Walk, Quenched Quantum Walk etc.

Mean exit times and extinction times: from TASEP to Population Dynamics

Estelle Pitard, Labaratoire Charles Coulomb, University of Montpellier, Montpellier, France

The dynamics towards absorbing states, such as the desintegration of a collection of particles, is adequately studied in the framework of out-of-equilibrium stochastic processes. In this talk, I will present two scenarios of interest, one in the context of transport, the other in the context of population dynamics. I will first address the question of the time needed by N particles, initially located on the first sites of a finite one-dimensional lattice of size L , to exit that lattice when they move according to a TASEP transport model. Then I will present results regarding the mean time to extinction of a population subject to birth and death processes in various spatio-temporal contexts of interest in ecology.

Unraveling the Mechanics of Z-Ring Formation and Stability

Debasish Chaudhuri, IOP Bhubaneswar, Bhubaneswar, India

The tubulin-like protein FtsZ is essential for cytokinesis in bacteria and archaea, forming the dynamic Z-ring at the division site. To elucidate its self-assembly, we develop a theoretical model treating FtsZ filaments as semiflexible polymers with defined mechanics and lateral attractions that stabilize ring structures. Molecular dynamics simulations reveal filament morphologies—open helices, chains, rings, and globules—capturing experimental observations in the fission yeast model using FtsZ from different bacterial species or mutants of *Escherichia coli*. The model captures how treadmilling activity governs Z-ring stability and identifies a spooling mechanism of assembly. At high activity, contractile and rotational stresses drive a transition to open helical states.

Differential motility leads to intestinal organoid budding

Anupam Gupta, IIT Hyderabad, Hyderabad, India

Intestinal organoids self-organize into complex crypt-villi architectures via spontaneous symmetry breaking. To understand the underlying biophysical mechanisms of the process, we developed a minimal agent-based model where motile, proliferative stem cells interact within a viscoelastic extracellular matrix, undergo fate decisions driven by YAP1–DLL1 signaling. Transient YAP1 activation induces DLL1 and Paneth cell differentiation, locally enriching Wnt3A. This creates motility and proliferation gradients, driving localized protrusions and sustained bud formation. Our results suggest that these spatial gradients in motility emerging from local fate decisions play a central role in driving mechanical instabilities that reshape tissue geometry. Complementarily, a

continuum model of a deformable elastic shell coupled to cell density revealed critical thresholds in motility strength and gradient length scale for bud formation, aligning with agent-based simulations. Our work defines a mechanistic phase space regulated by experimentally controllable biophysical quantities such as cell proliferation, motility, and YAP1 signaling heterogeneity, which collectively govern the onset of symmetry breaking and bud formation. This framework establishes a generalizable mechanochemical paradigm for morphogenesis, revealing how local cellular cues integrate with tissue-scale forces to orchestrate global shape transitions.

Decoding the grammar of multicomponent control of actin filament length: a theory-experiment dialogue

Sandeep Choubey, The Institute of Mathematical Sciences, Chennai, India

Actin is a cytoskeletal protein that dictates cell shape, motility, and intracellular transport. Its assembly and disassembly are tightly regulated by hundreds of actin-binding proteins that coordinate filament assembly and disassembly. While the functions of individual actin-binding proteins are well characterized, their combined effects on actin filament dynamics in vivo remain elusive. Advances in microscopy now enable precise, high-throughput measurements of filament lengths over time. However, these measurements remain largely underutilized owing to the lack of theoretical frameworks. To bridge this gap, we have developed a general kinetic model that captures the combined action of multiple regulatory proteins on actin dynamics. I will demonstrate how a dialogue between our theory and experiments have led to key insights into how cells control actin dynamics. Our approach reveals mechanistic insights that would otherwise remain hidden, paving the way for a deeper understanding of the grammar of multicomponent actin dynamics.

Fluid flow in 3-dimensional porous granular systems shows power law scaling with Minkowski functionals

Tapati Dutta, Physics Department, St.Xavier's College, Kolkata , India

Understanding flow through porous medium continues to be an active research area because of its important applications in our daily life - from subsurface flow important to agriculture, oil, and natural gas harvesting, CO₂ sequestration in sedimentary rocks to engineering applications, fluid transport in the pore space of a granular 3-dimensional structure is a complex non-linear problem. Transport of fluids in real situations, e.g., sedimentary rocks, is characterized by permeability or conductivity. However, these macro properties of the porous system are guided by micro to mesoscale properties like the size and shape of grains, which can have a wide distribution. Our work in this paper is inspired by Hadwiger's characterization theorem, which roughly says that the structure of finite unions of convex subsets of 3- dimensional systems can be described by at most four invariant measures - the Minkowski functionals. Therefore, it is not unreasonable to

expect that all transport properties, e.g., permeability, may be linked to the basic invariant geometric measures of the porous medium, as the grains can be assumed to be roughly convex. In this work we explore and develop a relationship between the four suitable Minkowski functionals and pore-scale properties of 3-dimensional systems. We systematically study the dependency of permeability on the geometrical characteristics of two categories of 3-dimensional porous systems generated: (i) stochastic and (ii) deterministic. For the stochastic systems, we investigated both normal and log-normal size distribution of grains. For the deterministic porous systems, we checked for a cubic and a hexagonal arrangement of grains of equal size. Our studies reveal that for any 3-dimensional porous system, ordered or disordered, permeability k follows a unique scaling relation with the four Minkowski functionals: (a) volume of the pore space, (b) integral mean curvature, (c) Euler Characteristic and (d) critical cross-sectional area of the pore space. The cubic and the hexagonal symmetrical systems formed the upper and lower bounds of the scaling relations, respectively. The disordered systems lie between these bounds. Moreover, we propose a combinatoric F that weaves together the four Minkowski functionals and follows a power-law scaling with permeability. The scaling exponent is independent of particle size and distribution and has a universal value of 0.43 for 3-dimensional porous systems built of spherical grains.

Dynamics of bacterial membrane sensing by antimicrobial peptides

Krishnakanth Baratam, The Institute of Mathematical Sciences, Chennai, India

Antimicrobial peptides, which work by disrupting the integrity of bacterial membranes, are of interest in the context of developing drugs for tackling multi-drug resistance. In this work, we examine this system from a physics perspective using molecular simulations. We aim to understand the dynamics of how an antimicrobial peptide interacts with the membrane, or vice versa, leading to the coupling of the membrane and the peptide. To achieve this, we employ a coarse-grained model of lipids and peptides to generate microsecond-scale molecular trajectories, which are then analysed using a variety of techniques to probe the mechanical and spatio-temporal properties of the membrane. The outcomes are put together to provide insights into the dynamics of the membrane and its modulation by the antimicrobial peptide.

q voter model with bias and disorder

Parongama Sen, Department of Physics, University of Calcutta, Kolkata, India

Collective decision-making is a process by which a group of individuals determines a shared outcome that shapes societal dynamics. A common approach to model these processes is using binary dynamics, where the choices are reduced to two alternatives. One of the most popular models in this context is the q -voter model, which assumes that opinion changes are driven by peer pressure from a unanimous group. We propose a generalized q -voter model that incorporates a bias towards one of the opinions. In this model, when the influence group is not

unanimous, the probability that an individual changes its opinion depends on the exact composition of the q-panel.

When the bias is neutral, the model is reduced to a mean-field voter model. We analyze the behavior and steady states of the system, identifying three distinct regimes based on the bias level: one favoring negative opinions, one favoring positive opinions, and a neutral case. In large systems, the equilibrium properties become independent of the size of the group, indicating that only the bias influences the final outcome.

Introducing a disorder in the form of contrarians in this model, analytical mean-field calculations and Monte Carlo simulations reveal that the final states of the system are governed by simple phase boundaries. Our findings highlight how contrarians, acting as structured non-conformists, can suppress consensus and maintain opinion diversity, while internal biases ultimately hinder a perfectly even split.

Triggering of Unstable slip in Sheared Granular Matter

Takahiro Hatano, Department of Earth and Space Science, Osaka University

The phenomenon of transient strain from seismic waves triggering earthquakes is a robust observation. However, our understanding as to why seismic waves can trigger earthquakes remains incomplete. In this study, we use particle simulations to investigate the response of sheared granular matter to dynamic strain perturbations in order to better understand the dynamic triggering of earthquakes. In our simulation, an unstable slip is triggered when the dynamic strain above a threshold is applied to the system. We show that the critical strain is of the same order as those in some experimental and observational studies. This enhanced response is observed at resonance wavelengths. Resonant vibration decreases the shear modulus of the granular system, and accordingly the shear strength is reduced, leading to unstable slip. This modulus softening is due to the increase in slipping contacts between particles. The relevance of simulation results to natural earthquake faults is discussed as to whether seismic waves can satisfy the resonance condition.

Non-equilibrium Dynamics in Fluids with Inhomogeneous Temperature Field

Sutapa Roy, Department of Physics, BITS Pilani-Hyderabad campus, India

Presence of temperature gradients give rise to interesting non-equilibrium phenomena which are not observed in isothermal fluids. Typical examples include Soret effect, large fluctuation-induced forces, etc. In this talk, we will present computer simulation results on the time-dependent structure formation in liquids with inhomogeneous temperature fields. Our findings from atomistic

molecular dynamics simulations and phase-field calculations will be compared to analytical predictions and experiments.

Fracture and plastic flow in disordered silica at the atomistic scale

Gaurav Singh, Department of Applied Mechanics, Indian Institute of Technology Delhi, New Delhi, India

In this talk, amorphous silica at atomistic scale will be considered as an archetypical disordered solid. I will first discuss how near crack tip stress field measurements may be made in crystalline (ordered) silicon before taking on amorphous (disordered) silica. Thereafter, I will justify at presence of plasticity in the near crack tip region before rigorously discussing the plastic flow in silica. Ree-Eyring equation, Drucker's postulate and convexity conditions will be demonstrated before a benchmark engineering problem using Ramberg-Osgood model.

From Fracture to Flow: Spatio-Temporal Dynamics and AI Insights in Drying Droplets

Anusuya Pal, University of Tokyo, Japan

Understanding how particles in complex fluids self-organize, experience stress, and interact during drying provides a powerful lens to explore far-from-equilibrium phenomena central to soft and multiphase systems. In this talk, I present a spatio-temporal study of microliter-scale biofluid droplets in diabetes, a metabolic disorder prevalent in South Asia, that evolve from dense crack networks to smooth, crack-free morphologies as they dry. These transitions arise from the interplay of capillary flow, solutal Marangoni circulation, and confinement-induced crowding, offering a soft-matter analogue to fracture dynamics and stress relaxation. By combining fluorescence imaging, optical profilometry, and particle image velocimetry with numerical modeling, I quantify how compositional heterogeneity and mechanical stress drive pattern evolution across scales. The resulting flow fields and 3D-profiles reveal a balance between Marangoni and capillary transport. Further, explainable artificial intelligence (AI) enables high-accuracy classification of the spatio-temporal dynamics during drying, linking emergent structures to their underlying physical mechanisms. This framework unites physics, biology, and data-driven approaches, highlighting drying droplets as model systems for studying such complex behavior. Although currently a proof-of-concept, the beauty of this approach lies in its simplicity—just drop, dry, and observe—revealing how fundamental physics with AI can address multidisciplinary challenges in diagnostics, sustainability, and beyond.

Linking Experimental Indices, Image Features, and Simulations of Soil Desiccation Cracks

V Madhurima, Department of Physics, Central University of Tamil Nadu, Thiruvavur, Tamil Nadu, India

Desiccation cracking in fine-grained alluvial soils significantly influences soil hydraulic properties, slope stability, and contaminant transport. This talk presents a comprehensive study combining experimental, analytical, and computational approaches to characterize and model crack formation in soils collected from the basins of Kaveri and Brahmaputra river basins. Laboratory experiments were conducted to evaluate swelling index and percolation rate under controlled drying–wetting cycles. The progression of crack networks was captured through imaging, followed by quantitative analysis using Minkowski functionals to extract measures of connectivity, shape, and anisotropy. In addition, supervised machine learning methods were employed to classify crack patterns and identify the soil types. To extend beyond laboratory scales, an agent-based modelling framework was developed to simulate the initiation, propagation, and interaction of desiccation cracks in heterogeneous alluvial deposits. The model accounts for soil-specific grain sizes, enabling comparative insights. By integrating experiments, image-based quantification, and computational modelling, this study provides a comprehensive understanding of desiccation crack dynamics in alluvial soils. The findings have direct implications for agricultural water management, floodplain engineering, and predictive modelling of soil behaviour under changing climatic conditions.

Prethermal Dynamics and Phase Synchronization in the Classical Kicked Rotor System

Tanay Nag, Department of Physics, BITS Pilani-Hyderabad campus, India

A many-body interacting system of classical kicked rotor serves as a prototypical model for studying Floquet heating dynamics. Having established the fact that this system exhibits a long-lived prethermal phase with a quasi-conserved average Hamiltonian before entering into the chaotic heating regime, we use spatiotemporal fluctuation correlation of kinetic energy as a two-point observable to probe the above dynamic phases [1]. We remarkably find the diffusive transport of fluctuation in the prethermal regime suggesting an underlying hydrodynamic picture in a generalized Gibbs ensemble with a definite temperature that depends on the driving parameter and the initial conditions. On the other hand, the heating regime is characterized by a diffusive growth of kinetic energy where the correlation is sharply localized around the fluctuation center for all time. Consequently, we attribute nondiffusive and nonlocalized structure of correlation to the crossover regime, connecting the prethermal phase to the heating phase, where the kinetic energy displays a complicated growth structure. We understand these numerical findings using the notion of relative phase matching where the prethermal phase (heating regime) refers to an effectively coupled (isolated) nature of the rotors. We exploit the statistical

uncorrelated nature of the angles of the rotors in the heating regime to find the analytical form of the correlator that mimics our numerical results in a convincing way. Going beyond the periodic drive, we consider here two types of aperiodic drives: random and quasiperiodic [2]. We observe a short-lived pseudothermal regime with algebraic suppression of heating for the random drive where WTD has an infinite tail, as observed for Poisson and binomial kick sequences. On the other hand, quasiperiodic drive characterized by a WTD with a sharp cutoff, as observed for the Thue-Morse sequence of kicks, lead to a prethermal region where heating is exponentially suppressed. We connect the synchronization dynamics with the above findings.

[1] A. Kundu, A. Rajak, Tanay Nag, Phys. Rev. B 104, 075161 (2021)

[2] A. Kundu, T. Nag, and A. Rajak, Phys. Rev. B 112, 064310 (2025)

Abstracts for Poster

Classical Annealing of Sherrington-Kirkpatrick Spin Glass Using Suzuki-Kubo Mean-field Ising Dynamics

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We propose and demonstrate numerically a fast classical annealing scheme for the Sherrington Kirkpatrick (SK) spin glass model, employing the Suzuki-Kubo mean field Ising dynamics (supplemented by a modified Thouless-Anderson-Palmer reaction field). The resultant dynamics, starting from any arbitrary paramagnetic phase (with local $m_i = \pm 1$ for the i^{th} spin, and the global magnetization $m = 0$), takes the system quickly to an appropriate state with small local values of magnetization (m_i) commensurate with the (frustrated) interactions. As the temperature decreases with the annealing, the configuration practically remains (in an effective adiabatic way) close to a low energy configuration as the magnitude of m_i 's and the spin glass order parameter q grow to unity. While the configuration reached by the procedure is not the ground state, for an N -spin SK model, the deviation in the energy per spin $E_N^0 - E^0$ is found to scale as $N^{-2/3}$, with $E^0 = -0.7629 \pm 0.0002$, suggesting that in the thermodynamic limit the energy per spin of the low energy configurations converges to the ground state of the SK model (analytical estimate being $E^0 = -0.7631667265 \dots$). Furthermore, the fluctuation σ_N in E_N^0 decreases as $\sim N^{-3/4}$ and the annealing time $\tau_N \sim N$, making this protocol highly efficient in estimating the ground state of the SK model.

Keywords: Ising spin glass, annealing, ground state energy optimization, SK-model.

Homogenization of Basal Topography Underlying Creeping Landmass: A Smoothed Particle Hydrodynamics Based Approach

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We investigate the slow-to-fast creep of landmass over a gentle slope by modeling the landmass as a weakly compressible viscous fluid. We specifically examine the influence of monochromatic basal topography on the run-out distance $r(\lambda)$, where λ is the wavelength of the topography over which the landmass creeps. We employ a mesh-free, Lagrangian approach using smooth particle hydrodynamics (SPH), treating the continuum as a collection of particles with local interactions. We consider a two-dimensional viscous flow on a gentle slope with an interparticle spacing of 0.08 m, generating approximately 3.13×10^5 fluid particles. The flow front consists of the region occupied by 30% of the particles at the leading edge, and the run-out distance, $r(\lambda)$, is defined as the averaged (weighted) coordinates of the particles in the front.

We found that creep propagation, for a given kinematic viscosity, exhibits a wavelength-dependent run-out distance, $r(\lambda)$. We determined that $r(\lambda)$ converges to the run-out distance $r(\lambda \rightarrow \infty)$, corresponding to planar topography, when λ is below λ_h and above λ_H . This provides upper and lower bounds on the topography wavelength λ , beyond which the topography has no influence on the creep run-out distance. We also identified a critical topography λ_m (where $\lambda_h < \lambda_m < \lambda_H$) at which the run-out distance reaches its minimum value. For a prescribed kinematic viscosity of $20 \text{ m}^2/\text{s}$, we found that $\lambda_H \sim 10^3 \text{ m}$ and $\lambda_c \sim 10 \text{ m}$.

Interfacial Slip Evolution with Causal Physics-Informed Neural Networks with Fourier Features

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Interfacial sliding is ubiquitous in geosciences, occurring in glacier beds, landslides, crustal faults, and subduction zones. Modeling approaches for interfacial slip evolution consider the medium to be elastically deformable and the interfacial strength to be dependent on sliding rate and its history. Here, we consider a machine learning approach to investigate slip evolution in an elasto-frictional, single degree of freedom, system. Specifically, we explore how physics-informed neural networks and their variants simulates evolution of slip and shear stress during inter-seismic, pre-

seismic, co-seismic and post-seismic stages. The mapping of continuous systems to a single-degree-of-freedom system is accomplished using the equivalent stiffness approach.

We highlight that the Causal Physics-Informed Neural Network (C-PINN) framework captures the rapid transition towards slip-instability that precedes the onset of dynamic sliding rates. Further, we use Fourier Feature embeddings in the input layers to avoid classical spectral bias that usual coordinate-based neural networks suffer. We maintain temporal causality by sequential training. We used hyperbolic tangent (tanh) activation function and hyper-parameters are optimized with the L-BFGS algorithm to ensure stable and rapid convergence. We show that the C-PINN based approach to solve for interfacial slip and shear stress resembles classical numerical solutions. We found that incorporating Fourier feature embeddings, compared to naive PINNs, improves the model's ability to capture rapid slip rate transitions.

Emergence of soft dynamic channels in highly ordered lipid bilayers

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Over the last few decades, extensive investigations on spatial and dynamic heterogeneity in plasma membrane (PM) have been performed on carefully reconstituted membranes. Characterizing the molecular features in heterogeneous membranes is extremely challenging due to experimentally inaccessible time- and length-scales of these emergent systems. In this context, simulations can provide important insights into molecular-level interactions leading to PM heterogeneity and associated functions. To that end, we use the non-affine displacement (NAD) framework [1] to faithfully capture molecular-scale local membrane order in simulated heterogeneous bilayers. In our latest application of NAD, we investigate the temperature-dependent spatial and temporal organization on microsecond trajectories of liquid-ordered bilayer systems at all-atom resolution (DPPC/DOPC/CHOL: 0.55:0.15:0.30; 40 nm x 40 nm with a total of 5600 lipids and 2 million atoms) [2]. Lateral organization in these large bilayer patches shows noticeable heterogeneity despite its liquid-ordered nature. Our analyses reveal soft dynamic channels within the tightly packed membrane reminiscent of the classical two-component Kob-Andersen glass-forming binary mixture. Hence, we quantified the multiple time scales underlying the lipid dynamics using classical glass physics markers such as self intermediate scattering function, dynamic susceptibility, van Hove etc., Our analyses reveal that highly ordered membrane systems inherently possess glass-like dynamics with distinct soft fluidic channels

inside them. Biologically, these soft fluidic channels could act as conduits for facilitating molecular encounters for biological functions even in highly ordered phases.

References:

1. Falk, M.L. and Langer, J.S., 1998. *Physical Review E*, 57(6), p.7192.
2. SureshKumar, H., Iyer, S.S., Banerjee, A., Poduval, P., Lyman, E. and Srivastava, A., 2025. *The Journal of Chemical Physics*, 162(14).

Experimental and Agent-Based Modeling of Soil Percolation Using NetLogo

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Based on experiments, it was observed that the percolation rate of water in soils depends on parameters such as soil type, particle size, pore structure, and particle packing. Experimental analysis of percolation was carried out for clay, sandy clay, and sandy clay loam from Kaveri delta basin, laboratory under specific boundary conditions. With only a limited number of trials performed, the results varied significantly across trials, showing no consistent trend for each soil type.

To address the limitations of conducting a large number of physical trials, agent-based modelling (ABM) simulations using *NetLogo* software. The different soil types were modelled as different particle sizes. The simulations showed that results still varied significantly across trials. Histograms of wet percentage indicate varied distributions types for each soil type depending on their percolation threshold. The results of ABM help in understanding the inconsistent experimental results, establishing the need for a much larger sample size for experiments in soil percolation.

Coffee Ring Effect of Soil Suspensions

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The coffee-ring effect, which occurs when an aqueous droplet of suspension evaporates on a substrate, can segregate suspended nanoparticles by size due to geometric constraints at the contact line. This study investigates this phenomenon in suspensions prepared from ball-milled soil samples and nano-clays. Experiments were conducted on two nano-clays, Halloysite (kaolin-group clay) with a tubular structure and Montmorillonite (bentonite) with a platelet-like structure. Soils under study are classified as clay, silt, sandy clay and sandy clay loam, based on the ratio of particle sizes. Soils were collected from two river basins, namely Kaveri and Brahmaputra. The soils from Kaveri are further classified based on the place of collection as left-bank (flooded) and right-bank (non-flooded). The coffee-ring formation for all samples were studied. The larger particles settle earlier and remain near the center, the intermediate particles settle around them, and the smaller particles flow outward and accumulate at the edge, forming a line. When the particles are uniform in size, they settle evenly and create a smooth surface; however, when the aqueous droplet contains a heterogeneous composition of particle sizes, this distribution changes. We report the characteristics of the different soils under study.

Efficient fluid extraction through hydraulic fracture in a capillary fiber bundle model

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Hydraulic fracturing, A process that enables the extraction of trapped oil and gas from shale formations by injecting high-pressure fluid into the subsurface. It has revolutionized hydrocarbon recovery from unconventional reservoirs by enhancing permeability. However, the process also carries risks, including induced seismicity and groundwater contamination, underscoring the need for more efficient approaches with minimal environmental impact. In this work, we investigate a one-dimensional capillary fiber bundle model subjected to a constant pressure gradient, incorporating stochastic fracking events. Each fracking event is modeled as a dynamic reduction in the threshold pressure of individual capillaries, representing the localized increase in pore space due to fracture formation. These events lead to a progressive enhancement in flow rate, reflected in the system's evolving rheology. Analytical solutions in certain limiting regimes show excellent agreement with numerical simulations, offering deeper insight into the underlying flow behavior. Our results reveal that the total volume of extracted fluid grows with the cumulative increase in pore space, and that the transition to linear Darcy flow occurs earlier due to fracturing. Importantly, we identify an optimal pressure gradient that maximizes extraction efficiency while minimizing risk, providing a quantitative basis for more effective hydraulic fracturing strategies.

Record statistics of emitted energies in the presence of crack and local stress concentration

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Reliable prediction of imminent catastrophic failure can aid in the mitigation of the damage caused by the collapse of infrastructure, such as buildings and bridges, and by natural disasters like landslides, avalanches, and earthquakes. Fracture in heterogeneous materials usually occurs in bursts or avalanches, which are usually accompanied by crackling noise that can be captured in acoustic emission (AE) experiments. These crackling bursts become more populated and exhibit an onset of acceleration as the system progresses towards catastrophic failure. A similar behaviour has also been observed in the record statistics of the energies emitted during these bursts. It has also been seen that the lifetime of the record events of the burst signals reaches a maximum prior to the catastrophic failure, thereby serving as a reliable predictor for imminent failure of the system.

In this work, controlled numerical simulations have been carried out in a statistical model for fracture, known as the fiber bundle model. The record statistics of emitted energies is studied with the addition of two new parameters : (i) the inclusion of a pre-existing crack of length l and (ii) a stress relaxation range γ to control the local stress concentration. Through a study of the Pearson correlation function, a phase diagram on the crack length vs stress relaxation range plane is drawn which demarcates the region where reliable prediction of imminent failure is possible from the region where it is not possible.

Investigating Mechanics of Fibrin via Elastic Network Modeling

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Fibrin is the principal structural protein of a blood clot that forms in response to hemostasis. It exhibits remarkable elasticity, strain-stiffening, and mechanical toughness in response to both tensile and shear deformation forces. The hierarchical assembly of fibrin from fibrinogen monomers to protofibrils has been extensively studied, but fibrin mechanics is still very poorly understood. In this regard, we employ Anisotropic Elastic Network Models to first identify modes and hinge regions of the fibrinogen monomer that dictate deformation pathways in response to applied mechanical load. Our objective is to integrate our findings into a coarse-grained framework that can provide a basis for simulating molecular-scale deformation under cyclic applied load, that helps explain the resultant fibrin fiber extension and strain stiffening properties.

Branching of fluid network in porous media

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The movement of fluid under the driving force at the interface between fluid and solid in porous media are ubiquitous in natural and industrial applications ranging from water uptake in plant roots to oil recovery, CO₂ sequestration, hydrogen storage etc. The shared characteristic among these flow systems, whether they are natural or industrial, is that their structure is being modified with the specific objective of enhancing flow accessibility. The development of flow configurations occurs due to an increase in flow rate with increasing resistances, achieved by altering the diameters and lengths of channels as well as through branching, all while maintaining a constant fluid volume. In these domains, predicting the amount of fluid that the network can extract by capillary movement is of paramount importance. In the current work we investigate the dynamics of branching during a two-phase flow of immiscible fluids under an external applied pressure P combined with the inherent capillary force in the branches with decreasing radius. The rheology of the flow will be studied with the branching ratio, the ratio of the radius of the two branches at a branching point, to control the directionality of the flow from the source to the outlet.

Enhancement in the mechanical properties of PVA-MoS₂ QD composite: An experimental and numerical study

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Nanoparticle-infused composites show improved structural and mechanical properties, attracting interest in the materials and aerospace industries. This study investigates the effect of incorporating hydrothermally-synthesized [Crystal Growth 627, 127487 (2024)] molybdenum disulfide quantum dots (QDs) into polyvinyl alcohol (PVA) to improve toughness of the composite [Polymer Bulletin 72, 2033 (2015)]. Here, PVA sheets with varying QD concentrations were subjected to tensile strength test. The concentration is varied from 73mM to 438mM prepared in a 2% PVA solution. The results revealed a notable degree of plastic deformation and elongation at an intermediate concentration of the QDs. Non-monotonic behavior has been observed in the toughness value for the sample 219mM, indicating reduced toughness for pure PVA, as well as for both lower and higher QD concentrations. This experimental study is followed by numerical simulation using the fiber bundle model [Physica A 627, 129129 (2023)], where different concentration is represented by varying elasticity values across the different systems. The model mimics failure event through a number of avalanches triggered through threshold activated dynamics. Experimental results align with simulations, showing that the extent of the plastic region exhibits the same non-monotonic behavior with maximum toughness, and relatively stable avalanche dynamics coinciding at the same point.

Pressure driven capillary rise dynamics.

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The present investigation aims to fundamentally elucidate the dynamics of capillary-driven flow in fibrous porous media under an externally applied pressure gradient using COMSOL Multiphysics. A two-dimensional axisymmetric model was developed within the Porous Media and Subsurface Flow module, coupling Darcy's Law with phase transport equations to simulate two-phase (liquid–air) flow through a compressed fibrous structure. The Brooks–Corey model was implemented to define the capillary pressure–saturation relationship and relative permeabilities, while experimentally measured parameters such as porosity, permeability, surface tension, and contact angle were incorporated into the model. Transient simulations were performed to track the evolution of pressure, velocity, and saturation fields within the domain. The analysis focuses on quantifying how variations in the applied pressure head modify infiltration rate, liquid front propagation, and internal pressure distribution compared to purely capillary-driven cases. This approach establishes a computational framework to predict and control capillary flow behaviour in fibrous media, providing physical insight and numerical validation relevant to industrial filtration, drying, and biological transport systems.

Phase Separation in Fluids with Inhomogeneous Temperature Fields

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Upon quenching an initial homogeneous fluid to a temperature below the critical temperature, it phase segregates and forms domains which grow with time. Such domain growth dynamics are rarely studied in the presence of inhomogeneous temperature fields. Using numerical calculations, we will present results for domain growth in the presence of temperature gradients.

Interfacial Slip Evolution with Causal Physics-Informed Neural Networks with Fourier Features.

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Interfacial sliding is ubiquitous in geosciences, occurring in glacier beds, landslides, crustal faults, and subduction zones. Modeling approaches for interfacial slip evolution consider the medium to be elastically deformable and the interfacial strength to be dependent on sliding rate and its history. Here, we consider a machine learning approach to investigate slip evolution in an elasto-

frictional, single degree of freedom, system. Specifically, we explore how physics-informed neural networks and their variants simulate evolution of slip and shear stress during inter-seismic, pre-seismic, co-seismic and post-seismic stages. The mapping of continuous systems to a single-degree-of-freedom system is accomplished using the equivalent stiffness approach.

We highlight that the Causal Physics-Informed Neural Network (C-PINN) framework captures the rapid transition towards slip-instability that precedes the onset of dynamic sliding rates. Further, we use Fourier Feature embeddings in the input layers to avoid classical spectral bias that usual coordinate-based neural networks suffer. We maintain temporal causality by sequential training. We used hyperbolic tangent (tanh) activation function and hyper-parameters are optimized with the L-BFGS algorithm to ensure stable and rapid convergence. We show that the C-PINN based approach to solve for interfacial slip and shear stress resembles classical numerical solutions. We found that incorporating Fourier feature embeddings, compared to naive PINNs, improves the model's ability to capture rapid slip rate transitions.

Inequality of Earthquake energy releases

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Earthquake prediction remains one of the most difficult problems in geophysics and statistical physics. In our work, we explore a new approach using statistical inequality measures—the Gini and Kolkata indices—to detect subtle changes in stress distribution before failure. Using two model systems—a 1D train model and a 2D sandpile-like earthquake model—we observe that these indices show distinct precursory variations prior to major avalanches. The ROC analysis, with an area under the curve of about 0.8, confirms the predictive prospects of these methods. This suggests that inequality measures, often used in economics and social systems, can also serve as potential indicators of criticality in natural systems.

Molecular Rewiring and Compensatory Mechanisms Sustain DNA Recognition in Mutant ZTA Transcription Factor related to Epstein-Barr virus: Insights from molecular dynamics simulations

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Protein–DNA complexes are stabilized by multiple non-covalent interactions such as hydrogen bonds, electrostatics, van der Waals forces, and hydrophobic contacts that together form a dynamic interaction network. Any perturbation, such as mutation or conformational change, can

reorganize this network and alter structural stability. To investigate this rewiring mechanism, we performed all-atom molecular dynamics simulations, binding-energy decomposition, and biased sampling on the Epstein–Barr virus (EBV) Zta transcription factor–DNA complex. Wild-type and mutant systems were studied by replacing a key positively charged arginine residue with oppositely charged glutamic acid. The substitution disrupted original interactions but led to the formation of new compensatory ones. Analysis of unbiased MD trajectories revealed that other residues, either within the same Zta monomer or across monomers, dynamically reorganize their contacts to counterbalance the lost interactions, thereby maintaining overall stability. However, multiple mutations exceeded this compensatory capacity, resulting in structural destabilization. Time-dependent hydrogen-bond analyses highlighted the role of transient contacts in stabilization, while dynamic cross-correlation mapping captured residue communication and motion coupling. Together, our results provide mechanistic insight into charge-dependent interaction-network reorganization in Zta–DNA systems, offering broader implications for understanding BZIP family transcription factors and for designing therapeutic strategies against EBV.

Modeling and Analysis of Electroosmotic Pump Flow Dynamics for High Heat Flux Cooling Space Applications

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Electroosmotic pumps (EOPs) have gained considerable attention as compact and efficient devices for thermal management in high heat flux electronic systems. These pumps operate through electrokinetic transport within micro- and nanochannels, where the interaction between ionic motion, electric fields, and viscous forces produces complex nonlinear flow characteristics. Understanding these coupled processes requires a combination of statistical and continuum-level modelling to capture charge transport, potential distribution, and fluid motion accurately.

In this study, the electroosmotic flow behaviour is analysed using the coupled Poisson–Nernst–Planck and Navier–Stokes equations. The model provides insights into how zeta potential, applied electric field strength, and channel geometry influence flow rate and pressure generation. The investigation highlights the critical role of interfacial charge distribution and the nonlinear effects of the electric double layer in determining the overall pump performance.

The outcomes contribute to a deeper understanding of electrohydrodynamic transport in microfluidic systems and offer guidance for optimizing design parameters for efficient heat transfer space applications. This work bridges the gap between theoretical modeling and practical implementation by linking microscale electrokinetic effects to macroscale flow and thermal performance, ultimately aiding the advancement of next-generation space cooling technologies based on electroosmotic flow.

Tailoring Co-Ni Nanoclusters on Graphene-Based Supports for Enhanced Electrocatalysis: A Descriptor-Based Approach to Cost-Effective Catalyst Design

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Finding the correct descriptor for nanocluster-based systems, particularly for oxygen evolution reaction is a great challenge because as we move into the domain of nanoclusters the electronic properties of metal sites can vary significantly depending on their local environment. Therefore, till now the mechanisms driving the high activity and selectivity of nanocluster-based systems, particularly those supported on graphene, remain complex and difficult to explain. Our research addresses this challenge by focusing on cobalt (Co) and nickel (Ni) nanoparticles of varying sizes supported by graphene, exploring their catalytic activity in relation to d-orbital-based electronic descriptors. These transition metals are not only abundant and cost-effective but also exhibit promising OER activity. After, density functional theory-based screening of more than 130 metal sites of Co and Ni nanoclusters we have found out that 19Ni nanoparticle was the most favourable system with 0.44V overpotential among 41 systems. Despite recent advancements, there remains a need for an effective electronic descriptor that can accurately predict and explain OER performance, enabling the identification of optimal compositions and active sites. To meet this need, we have developed a predictive model based on d-band descriptors using ML, extending the success of such models from carbon-based, metal-free systems to metal nanoclusters^{1,2,3}. By correlating d-band properties with catalytic performance, we aim to systematically identify promising materials and active sites, reducing reliance on costly and time-consuming trial-and-error methods in both experimental and computational studies. This research has the potential to significantly accelerate the discovery of high-performance electrocatalysts, making the development process more efficient and cost-effective. Ultimately, our work contributes to the broader goal of designing next-generation materials for clean energy technologies at low cost.

The phase transition in the Vicsek model through Gini Index

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At the critical point of a phase transition, the fourth-order Binder cumulant (U), which is a measure of departure from Gaussianity in the order parameter, becomes independent of the system size and obeys a finite-size scaling relation with the correlation exponent. This feature has been widely used to estimate the critical point and exponents accurately from simulations. Recently, the Gini index, a measure of inequality that traditionally is used in economics to quantify wealth inequality,

has been shown to be useful for studying phase transitions in physical systems at equilibrium. By studying phase transition in equilibrium, it has been numerically demonstrated that at the critical point, g in the order parameter becomes independent of the system size and follows a finite-size scaling relation similar to U . Here, we investigate the nonequilibrium phase transition in the Vicsek model [1] of active systems in two dimensions using the index g . For this model, we find that both g and U exhibit similar behavior. For a high self-propelled velocity, both g and U are system size independent at the critical point and obey a finite-size scaling relation for the correlation length exponent. For small self-propulsion, we find the transition is unusual, as there is no single point where g (or U) for various system sizes crosses.

[1] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, Physical review letters 75, 1226 (1995)

Experimental and Agent-Based Modeling of Soil Percolation Using NetLogo

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Based on experiments, it was observed that the percolation rate of water in soils depends on parameters such as soil type, particle size, pore structure, and particle packing. Experimental analysis of percolation was carried out for clay, sandy clay, and sandy clay loam from Kaveri delta basin, laboratory under specific boundary conditions. With only a limited number of trials performed, the results varied significantly across trials, showing no consistent trend for each soil type.

To address the limitations of conducting a large number of physical trials, agent-based modelling (ABM) simulations using NetLogo software. The different soil types were modelled as different particle sizes. The simulations showed that results still varied significantly across trials. Histograms of wet percentage indicate varied distributions types for each soil type depending on their percolation threshold. The results of ABM help in understanding the inconsistent experimental results, establishing the need for a much larger sample size for experiments in soil percolation.

Role of activity and dissipation in achieving precise beating in cilia: Insights from the rower model

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Cilia and flagella are micron-sized filaments that actively beat with remarkable precision in a viscous medium, driving microorganism movement and efficient flow. We study the rower model to uncover how cilia activity and dissipation enable this precise motion. In this model, cilia motion is represented by a micro-beads Brownian movement between two distant harmonic potentials. At specific locations, energy pumps trigger potential switches, capturing cilia activity and generating oscillations. We quantify precision of oscillation using a quality factor, identifying its scaling with activity and oscillation amplitude, finding precision maximization at an optimal amplitude. The data collapse is not accurate for noisy oscillations. An exact analytic expression for the precision quality factor, based on first passage time fluctuations, and derived in the small noise approximation, explains its optimality and scaling. Energy budget analysis shows the quality factor's consistency with the thermodynamic uncertainty relation.

Quantum walk without wavefunction: A classical interacting particle model

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We explore a stochastic framework that connects discrete-time quantum walks (DTQWs) with a classical interacting particle (CIP) model, aiming to understand quantum transport phenomena as emergent from collective classical dynamics. In this approach, a large but finite number of interacting particles evolves through nonlinear update rules, mimicking the coin and shift operations of the DTQW. Without invoking any wavefunction, effective quantum-like behavior arises solely from the nonlinear interactions between these particles. By framing the DTQW within the language of interacting stochastic processes, this study bridges classical and quantum descriptions of diffusion and transport, offering new insights relevant to complex systems and non-equilibrium dynamics.

Unraveling ligand dissociation pathways through path classification algorithms

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The knowledge of ligand dissociation pathways and their associated kinetics together with binding affinity play crucial role in determining ligand efficacy and selectivity. Predicting dissociation pathways for ligand-protein, DNA-protein systems are challenging from conventional molecular dynamics due to limitations in length and time scales. Here, using enhanced sampling technique, OPES-explore, a variant of OPES (on-the-fly probability enhanced sampling), we sample the ligand dissociation pathways. From the derived high- dimensional time series trajectories, selecting an appropriate similarity/dissimilarity measure and a suitable clustering algorithm, we predicted dissociation pathways for different model potential and real protein-ligand systems and performed a comparative study in selecting efficient method.

Keywords: Dissociation pathways, OPES-explore, similarity measure, clustering algorithms.