Invited Talks

Mechano-chemistry drives shape transformation in cells

Anirban Sain
IIT Bombay

All living cells undergo change in shape during its growth, division and differentiation. Many of these processes can be understood in terms of mechanics at a mesoscopic scale. This requires invoking elasticity and fluidity of the cell membrane and cell wall at micron scales and describing cellular dynamics using the language of force, stress and energy. In this description role of the underlying molecular level processes are considered in terms of their integrated effect on local stresses. I will describe two such examples, namely, cell division in animal tissue and sporulation in bacteria, with an attempt to identify universal aspects in each of these subclasses.

Criticality in Cell Differentiation

Indrani Bose
Bose Institute Kolkata

Cell differentiation is a key biological process in which stem or progenitor cells diversify into different cell types, e.g., blood, skin, kidney, liver cells etc. Recent experiments on blood cell differentiation in mice have identified some distinctive features of the undifferentiated cell population on the verge of differentiation. These are: a considerably broad heterogeneity was observed in the distribution of a key protein in the ensemble of cells, the protein distributions in the subpopulations sorted from the parental cell population were found to regain the parental distribution, in fresh growth medium, through slow kinetics over a period of two weeks and lastly, the different subpopulations of the undifferentiated cell population have different propensities for lineage choice (multilineage priming) once differentiation sets in. In this talk, an elementary introduction will be given to the computational and mathematical approaches for identifying the physical principles underlying cell differentiation. Our mathematical model provides an explanation of the experimentally observed features based on the proposal of criticality, i.e., proximity to a critical point. The talk will illustrate how the concepts of maximum entropy principle and phase transition from statistical physics provide a new physical understanding of the biologically important process of cell differentiation.

Understanding molecule-molecule associations in cell orchestra : Complex network framework

Sarika Jalan
IIT Indore

The inside of a cell is turbulent with activity, as enormous proteins, tiny molecules, and DNA strands wind around each other to accompany thousands of interactions. Each of these molecules is a set of functioning assistants of other molecules that helps in the proper cellular signaling. Hence, the overall functioning of these molecules is of jugglers play in the cell orchestra. The functioning of the cell can take on a very different character if even a single member of this molecular orchestra starts to behave strangely. The effects of wave apparent from the primary flaw, causes problems i.e. disease on the system level. The disease state is a consequence of one or many of such flaws in molecular interactions that eventually result in the altered dynamics of the expressions of infected molecules. Understanding the relationship between these altered molecular interactions resulting in the altered molecular pathways based on the underlying biological mechanisms is one of the greatest challenges in modern biology and medicine.

Development of statistical tools inspired from other branches of sciences particularly from graph theory and random matrix theory enables us to have a global view of the diseasome. These tools uncover the complexity of the disease and understand disease at the fundamental level. This talk explores molecule-molecule associations through the holistic combined framework of the systems biology approach, network theory and random matrix theory is expected to trace differences in the associations of normal and disease states and improve our current knowledge of molecular associations in diseases, which may principally lead to further much required improvements in health care of disease diagnosis, progno sis and treatment.

Dynamics of Cytoskeletal filaments

Ranjith Padinhateeri
IIT Bombay

Tubulin and actin are cytoskeletal proteins that dynamically polymerize and depolymerize to take part in many important functions in the cell that include cell motility and cell devision. These proteins are also among the simplest ”molecular machines” that use chemical energy and perform mechanical work. We will discuss how use statistical physics to investigate dynamics of these filaments and their collective effects.

Lessons from a feed forward and feedback network in olfactory pathway

Joby Joseph
University of Hyderabad

In neuronal systems we can come across feed forward motifs with large convergence and feedback motifs. In this talk we will look at an example each of these circuit motifs. Spontaneous activity is present in the neurons in different parts of the brain. Some of these are endogenously generated activity of the system (like in the case of pacemakers and recurrent loops for memory consolidation), some are involved in maintenance of short term memories, while some of these spontaneous activities are considered as noise in the system. Part of this noise is contributed by unreliable mechanisms at synaptic and transduction machinery or at the cell membranes of neurons in the organism. Organism has evolved different strategies to perform in the presence of this noise. In the olfactory pathway in insect systems it is observed that there is relatively high levels of spontaneous activity in the sensory neurons and the second order neurons (called projection neurons) to which all the receptor neurons of same type converge. However the third order neurons (Kenyon cells) that these converge to are eerily silent and yet sensitive to odors at very low concentrations with sparse coding at high concentrations. We combine experiments and simulations to address some of the following questions. Is the spontaneous activity in the second order neuron caused by the receptor neurons? Why is it not silent though there is convergence to it from all the receptor neurons of identical types? How is it that the third order neurons maintain very low spontaneous activity while they are able to respond stably to odors ranging from very low to very high concentrations?

Computational methods for analysing neuroimaging data

Krishna Prasad
IIT Gandhinagar

I will discuss methods of experimental design, physics of MRI, data analysis procedures using statistical parametric mapping, functional connectivity analysis, multivariate pattern analysis using machine learning techniques, and data mining approaches for brain imaging.

Big Data from Single Cells - Addressing Statistical and Computational Challenges

Saumyadipta Pyne
IIPH Hyderabad

Systems Biomedicine is an emerging approach to address issues of complexity and heterogeneity that underlie large biological datasets generated using increasingly higher resolution and higher throughput platforms. Yet, if one is ready to accept these challenges, then it is possible to try to understand diseases as states that result from the perturbation of biological systems, often modeled as multi-level networks that can propagate effects from single molecules to complex pathways, and indeed, to the level of entire mechanisms and even species. Towards this, our aim is twofold: first, to study some of the complex systems in fine resolution, and to do that, we have devised analytical platforms that can model the dynamic and stochastic behavior of biological samples at the single-cell level. This allows us to monitor and precisely model transitions of cellular states as they differentiate, send certain signals or respond to various conditions. Secondly, we have developed statistical methods to test the effects of lower level or early stage modulation of developmental and pathological processes in terms of outcomes that are measurable at higher levels or later stages in the system. Our work has been applied to studies of cancer, immunology and regenerative medicine.

Computational Protein Design

Pralay Mitra
IIT Kharagpur

Computational protein design is a reverse procedure of protein folding and structure prediction, where constructing structures from evolutionarily related proteins has been demonstrated to be the most reliable method for protein three-dimensional structure prediction. Following this spirit, we developed a novel method to design new protein sequences based on evolutionarily related protein families. For a given target structure, a set of proteins having similar fold are identified from the Protein Data Bank by structural alignments. A structural profile is then constructed from the protein templates and used to guide the conformational search of amino acid sequence space, where physicochemical packing is accommodated by single-sequence based solvation, torsion angle, and secondary structure predictions. The method was tested on 87 protein structures covering different fold classes and 243 structurally resolved proteins in the pathogenic bacteria Mycobacterium tuberculosis. The experimental evidences for five randomly picked designed proteins showed solubility with distinct secondary structure and three have well-ordered tertiary structure, as demonstrated by circular dichroism and NMR spectroscopy.

Short Talks

A New Similarity Measure for Identification of Disease Genes

Ekta Shah
ISI Kolkata

One of the important problems in functional genomics is how to select the disease genes. In this regard, the paper presents a new sim- ilarity measure to compute the functional similarity between two genes. It is based on the information of protein-protein interaction networks. A new gene selection algorithm is introduced to identify disease genes, integrating judiciously the information of gene expression profiles and protein-protein interaction networks. The proposed algorithm selects a set of genes from microarray data as disease genes by maximizing the rel- evance and functional similarity of the selected genes. The performance of the proposed algorithm, along with a comparison with other related methods, is demonstrated on colorectal cancer data set.

Integrated Data Analysis Using Rough Hypercuboid based Canonical Correlation Analysis

Ankita Mandal
ISI Kolkata

One of the major problems in real life data analysis is how to extract features from multimodal high dimensional data sets, which are relevant and nonredundant. To extract new features from multimodal omics data sets, the supervised regularized canonical correlation analysis, which plays an important role, optimizes regularization parameters based on the quality of first pair of canonical variables only using standard feature evaluation indices. In this regard, a new SRCCA algorithm is proposed based on SRCCA and rough hypercuboid approach, to extract relevant and nonredundant features in approximation spaces from multimodal multidimensional omics data sets. Rough hypercuboid approach provides an efficient way to calculate the degree of dependency of class labels on feature set in approximation spaces, while SRCCA helps in extracting nonredundant features from multimodal data sets.

Analysis of a virus dynamics model with saturated infection rate and immune response in presence of therapeutic drug

Preeti Dubey
BITS Pilani

Virus dynamics models are important source of information for research of emerging diseases like SARS, Ebola, Influenza, HIV/AIDS, hepatitis B & C etc. Here, we studied the role of immune response and therapeutic drug to understand the dynamics of uninfected cells, infected cells and free viruses. A threshold value of basic reproduction number of infection in presence of immune response (RI) is established. Further, global stability of virus free equilibrium and interior equilibrium is discussed analytically using LaSalles principle and Lyapunov Direct method. Central manifold theory is used to study the dynamics of equilibrium points near RI =1: A special case, when the immune response is absent, has also been studied. Numerical simulations are performed to validate the analytical results using MatLab and Mathematica.

Bribe and Punishment: An Evolutionary Game-Theoretic Analysis of Bribery

Prateek Verma
IISER Kolkata

Harassment bribes, paid by citizens to corrupt officers for services the former are legally entitled to, constitute one of the most widespread forms of corruption in many countries. Nation states have adopted different policies to address this form of corruption. While some countries make both the bribe giver and the bribe taker equally liable for the crime, others impose a larger penalty on corrupt officers. We examine the consequences of asymmetric and symmetric penalties by developing deterministic and stochastic evolutionary game-theoretic models of bribery. We find that the asymmetric penalty scheme can lead to a reduction in incidents of bribery. However, the extent of reduction depends on how the players update their strategies over time. If the interacting members change their strategies with a probability proportional to the payoff of the alternative strategy option, the reduction in incidents of bribery is less pronounced. Our results indicate that changing from a symmetric to an asymmetric penalty scheme may not suffice in achieving significant reductions in incidents of harassment bribery.

Analysing behavioural response with generalized linear mixed models: a case study on social wasp colonies

Paromita Saha
IISc Bangalore

Quantification of behaviours is essentially based on sampling. As behaviours are ephemeral, the datasets often turn out to be non-normally distributed which makes them inappropriate for applying basic parametric statistics that rely on normal distribution. Moreover, both observational studies and controlled experiments in behavioural ecology often involve nested design where sampling blocks are replicated over space and time. Generalized linear mixed models (GLMM) offer a simultaneous solution to both the problems by combining two statistical frameworks- generalized linear models for handling non-normality and linear mixed models to take care of the repetitive data structure by incorporating random effects. Here we present a case study conducted on the Indian paper wasp colonies. A typical colony is composed of a reproductively active queen and several functionally sterile workers. This queen is periodically replaced by one of her workers. We were interested in behavioural response of this succeeding new queen. Therefore we opportunistically observed 11 natural colonies during queen turnover and experimentally removed the existing queen in 9 colonies. In both the cases we recorded aggressive bevariours shown by all the individuals before and after the original queen is lost. This dataset was found to follow negative binomial distribution. GLMM appeared to be the best approach for analyzing the pattern of aggressive behaviours shown by the new queen across natural and experimental colonies, where the individual wasp identity and their colony identity were considered as nested random effects.

Meta-analysis of gene expression microarrays to understand plant defenses during pathogen attack

Avinash Sethi
IISER Kolkata

A major challenge in systems biology is to perform integrative analysis of large-scale datasets that are obtained from various high-throughput studies as well as from the use of variable platforms. One such technique that allows rapid generation of data is the gene expression microarrays. For combining the results from a variety of microarray studies in plants, we present a methodical framework for the meta-analysis for determining differentially expressed genes obtained from such datasets. The framework is evaluated and applied in transcriptomics DNA microarray data to elucidate rewiring of gene expression during powdery mildew infection in plants. Complex reprogramming during the course of infection involves 5350 genes in Arabidopsis thaliana. Largest group of genes showing elevated expression during infection cycle comprises of transcriptional regulators, phytohormone signalling pathways and secondary metabolic pathways. Generalized as well as species specific signatures of responses and underlying molecular mechanisms are elucidated to reveal complex regulatory network underlying plant pathogen interactions. Our study presents an example of how to determine overlapping and unique responses in model organisms vs. agriculturally important crops.

Posters

1. **Effect of A. . .A mismatch in a CAG trinucleotide repeat overexpansion: a comparative study of DNA force fields**
   Aditya Kr. Sarkar

2. **Characterization of ul18 glycoprotein of HCMV and Class I MHC molecule homology through the pattern based analysis: an in-silico approach**
   Agniswar Sarkar, ICMR Virus Unit
3. **Cold environment is a greater risk of cancer for females: A county wise study of USA**
   Ankit Sharma , Cenral University Rajasthan
4. **Elucidating the DNA binding characteristics of basic-region leucine zipper (bZIP) proteins**
   Anwesha Sarkar, University of Calcutta
5. **Estimation of mean first passage time for bursty gene expression.**
   Anudeep Surendran & Mayank Shreshtha , IISER Kolkata
6. **Understanding Disease Networks through Protein-Protein Interactions**
   Aparna Rai , IIT Indore
7. **Virtual analysis for the structural and functional charecterization of pp65(ul83) tegument protein of HCMV with repect to different disease conditions.**
   Aroni Chatterjee, ICMR Virus Unit
8. **Decorrelation in neuronal systems enable better classification by neuron like elements**
   Bhavana Penmetcha, University of Hyderabad
9. **Collective cell migration during wound healing**
   Dipanjan Chakraborty & Abhilash Sahoo, IISER Kolkata
10. **Phylogeny of Metabolic Networks: A Spectral Graph Theoretical Approach**
    Krishanu Deyasi, IISER Kolkata
11. **Dogs on streets die young, thanks to humans: Early life mortality in free-ranging dogs**
    Manabi Paul, IISER Kolkata
12. **Assessing the Effects of Relative Infectiousness of HIV Positives and AIDS individuals on the intrinsic Dynamics of AIDS Epidemic**
    Manindra Kumar Srivastava , School of Management Sciences Lucknow
13. **Comparison of TFBS conservation in closely related Oryza species and its significance in identifying functional regulatory elements**
    Priya Rani Agarwal , University of Calcutta
14. **Emerging patterns in Biofilm formation**
    Rahul Kumar & Trinish Sarkar, IISER Kolkata
15. **Actin filaments growing against a barrier with fluctuating shape**
    Raj Kumar Sadhu, SNBNCBS
16. **An 'omics' approach to understand small-RNA mediated gene regulation in plants**
    Ravi Singh & Sangramjit , IISER Kolkata
17. **Stability of fixed points in S-metric spaces**
    Sabarni Debnath, Visvesvaraya National Institute of Technology
18. **Effect of Inactivating Mutations on Peptide Conformational Ensembles: The Plant Polypeptide Hormone Systemin**
    Saikat Dutta Chowdhury , University of Calcutta

19. **Relation between isochronicity and limi cycles for a two dimensional bio-chemical reaction model.**
Sandip Saha , SNBNCBS Kolkata

20. **Fine tuning of gain control in a negative feedback circuit.**
Shilpi Singh, University of Hyderabad

21. **Search process in E. coli Chemotaxis**
Subrata Dev, SNBNCBS

22. **Relation of Agglomerative Clustering and Topic Mapping on Neuro-imaging data**
Sujata Sinha, IIT Gandhinagar

23. **Comparative genomics and phylogenetic analysis reveal regulatory patterns of the Lysine riboswitch in bacteria**
Sumit Mukherjee, IISER Kolkata

24. **.**
Subhamoy Singha Roy, ISI/JIS

25. **.**
Vivek Rai , IIT Kharagpur