




1st IBSE International Symposium

From Genotype to Phenotype: Computational Approaches to Understand Biological Systems

IC&SR Auditorium, IIT Madras

<https://web.iitm.ac.in/ibse/symposium/>

The inaugural 1st IBSE International Symposium was organised from 22–24th January 2018 at IIT Madras. The symposium was inaugurated by the Director, IIT Madras, Bhaskar Ramamurthi who pointed out the importance of this symposium to not only usher in a transition from genotype to phenotype but eventually also to actionable prototypes. The Dean, International and Alumni Relations, R Nagarajan, talked about the importance and convergence of interdisciplinary activities in the campus and how IBSE is spearheading the interdisciplinary research in the biology domain.

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attendees had an opportunity to see the synergy between established companies and IITM as well as entrepreneurial ventures. Finally, the day ended with a banquet dinner at the Holiday Inn Chennai OMR IT Expressway Hotel.

On the second day, we had talks by Edda Klipp (Humboldt-Universitaet zu Berlin, Germany), Simon Anders (Zentrum für Molekulare Biologie der Universität Heidelberg, Germany), Shekhar Mande (NCCS, Pune), Niranjana Nagarajan (Genome Institute of Singapore), Manikandan Narayanan (Department of Computer Science and Engineering, IIT Madras), Erik van Nimwegen (Biozentrum, Basel, Switzerland) and Balaraman Ravindran (Department of Computer Science and Engineering, IIT Madras). Following the talks, we had an entertaining Carnatic music concert by *Kalaimamani* Smt Gayathri Girish. The final day of the symposium began with a stimulating talk by Giriraj Chandak (CCMB, Hyderabad), followed by Rudiyanto Gunawan (ETH Zürich, Switzerland), Vinod Scaria (IGIB, New Delhi), Amit Chaudhuri (MedGenome, Bangalore), and Haja Kadarmideen (Technical University of Denmark). The final talk was by Lars Steinmetz (EMBL Heidelberg, Germany; Stanford University, USA).

The day preceding the symposium, Rohit Gupta (MedGenome Labs Ltd, Bangalore) conducted a hands-on workshop and training on next-generation sequence analyses for the student participants. During the symposium, two poster flash talks and active poster sessions were the other highlights. At the end of the symposium, two poster prizes were awarded. The symposium was attended by students from all over the country, and a faculty each from IIT Guwahati and IIT Kharagpur. In the end, Rune Linding applauded our IBSE students' involvement and their energy at the symposium.

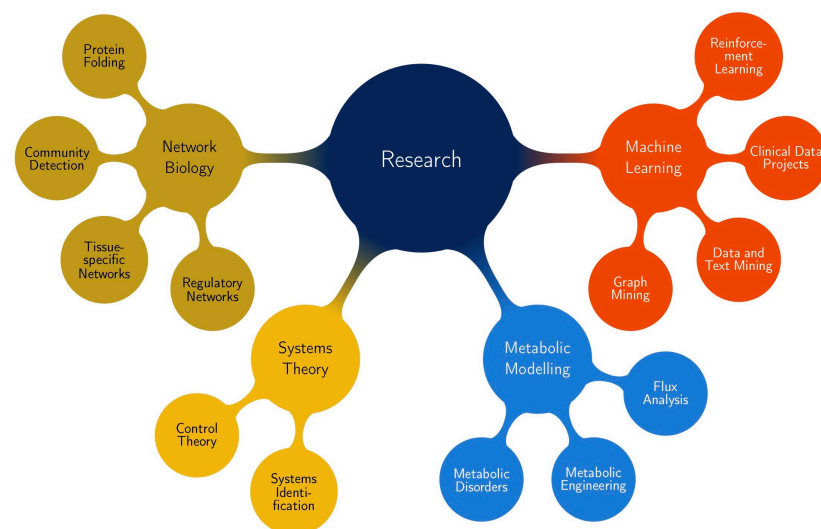
The organisers thank Dr Prakash Arunachalam, Lead Data Scientist, BNY Mellon, USA, for his generous contribution supporting the IBSE and funding this Symposium through the Office of International and Alumni Relations, IIT Madras. We also thank support from the Centre for Continuing Education and the Bhupat and Jyoti Mehta School of Biosciences, IIT Madras. The support of Prof Ashok Venkitaraman, Mehta Distinguished Chair (IIT Madras) and Director of MRC, University of Cambridge, UK, and Prof Bhaskar Ramamurthi, Director, Prof R Nagarajan, Dean, International & Alumni Relations, and Prof D Karunakaran, Head, Department of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences, IIT Madras, is gratefully acknowledged. Finally, we acknowledge the hard work of all IBSE student volunteers.

IBSE 1st International Symposium



Research

The interdisciplinary research at IBSE spans four main domains – Machine Learning, Network Biology, Metabolic Modelling, and Systems Theory. We have carried out some exciting work,



particularly in the area of biological networks and graph theory. RBCDSAI itself specialises in the study and analytics of networked data. IBSE has already produced some exciting results stemming out of the application of graph theory and network science to biology and (bio)chemistry, working on problems ranging from protein folding to the biosynthesis of biochemical compounds.

We have also used graph mining to learn the repertoire of chemical reactions that can occur in an organism and predicted new biochemical routes to synthesise metabolites. Very recently, we developed an efficient algorithm to enumerate all possible ways to synthesise molecules within a cell, or even across organisms, based on graph theory. Understanding these biochemical pathways enables us to predict new ways to synthesise chemicals for metabolic engineering, particularly in the bioprocess and pharmaceutical industries. We have successfully competed in “Disease Module Identification DREAM Challenge” to identify network modules for association with complex traits and diseases.

We also work on basic science projects that work towards enhancing our understanding of how cells function and how they can be (re-)designed. We also have ongoing studies that have helped us understand how redundancy and robustness evolve in biological systems, through computer simulations of metabolism. By drawing on systems theory, working with Chemical Engineers, we have been able to design biological circuits that show specific behaviours.

IBSE Faculty

Coordinators: Himanshu Sinha, Karthik Raman (Dept of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences), Ashok Venkitaraman (MRC, University of Cambridge, UK)

Core Faculty: Balaraman Ravindran, Manikandan Narayanan (Dept of Computer Science and Engineering), Raghunathan Rengaswamy, Swagatika Sahoo (Dept of Chemical Engineering)

Associated Faculty: Athi N Naganathan, Michael Gromiha, Nirav Bhatt (Dept of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences), Arun K Tangirala, Sridharakumar Narasimhan (Dept of Chemical Engineering), Sayan Ranu (IIT Delhi),

Adjunct Faculty: Rohit Gupta (MedGenome Labs Ltd, Bangalore)

Staff: Dr Philge Philip (IBSE)

Teaching

IBSE faculty offer a variety of interdisciplinary courses in the interface of biology, computer

science, and engineering.

Over ten undergraduates have already carried out their dual degree thesis projects in interdisciplinary areas with IBSE faculty, some even leading to publications. Also, over seven undergraduates are currently carrying out their thesis projects at IBSE.

IIT Madras has introduced Interdisciplinary Dual Degree (IDDD) programmes in several disciplines including Data Science. IBSE also contributes to this programme by offering courses as well as mentoring student projects. IBSE faculty also teach a module on “Big Data for Biology” in the Institute-wide undergraduate biology course – this further serves to attract budding engineers from across departments to work on challenging biological problems.

Courses offered by IBSE faculty

Data Structures and Algorithms for Biology (BT3051), Computational Systems Biology (BT5240), Quantitative and Population Genetics (BT5540), Systems Biology for Engineers (CH5016), Algorithmic Approaches to Computational Biology (CS6024), Multilayer Network Models and Algorithms (CS7012)

NPTEL Course: Computational Systems Biology (Jul-Oct 2018)

Collaborations and Partnerships

IBSE has active collaborations with research institutes viz. The Institute for Stem Cell Biology and Regenerative Medicine (inStem, Bangalore); National Centre for Biological Sciences (NCBS, Bangalore); Translational Health Science and Technology Institute (THSTI, Faridabad); National Institute for Research in Tuberculosis (NIRT, Chennai); and University of Sydney (through IIT Madras – University of Sydney Innovations in Biomedical Engineering and Medicine Research Alliance) and hospitals and clinics – Sankara Nethralaya (Chennai), Mohan's Diabetes Research Foundation (Chennai).

An agreement for the joint supervision of a doctoral degree between IBSE and Heidelberg University, Germany – “BioBigData” Cotutelle has been signed. IBSE is a non-EU partner in an EU Horizon 2020 Framework project “BIOROBOOST – Fostering Synthetic Biology standardisation through international collaboration”.

IBSE and RBCDSAI are data processing and analytics partners in “GenomeIndia: Cataloguing the genetic variation in Indians” – a multi-institutional project proposal to sequence 10,000 Indian genomes to represent the Indian genetic diversity with the aim to develop reference genome and genome-wide chip (GWAS) for genetic diagnosis at an affordable cost.



INITIATIVE FOR BIOLOGICAL SYSTEMS ENGINEERING
presents the inaugural lecture of the



IBSE COLLOQUIUM SERIES

What transcriptional noise tells us about the cell inside



Prof. Victor de Lorenzo is a chemist and Research Professor at the CNB-CSIC (Centro Nacional de Biotecnología, Spanish National Research Council) where he heads the Laboratory of Environmental Molecular Microbiology. He is a member of the EMBO, the American Academy of Microbiology and the European Academy of Microbiology.

He works at the interface of Synthetic Biology and Environmental Biotechnology.



Central Lecture Theatre

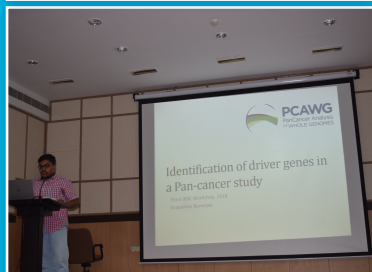
3.30 pm, 3 Nov 2017



IBSE Colloquium

The first of the IBSE Colloquium series was co-sponsored by EMBO and was conducted in November 2017. The inaugural speaker was Dr Victor de Lorenzo, Centro Nacional de Biotecnología, Spain, who talked about what transcriptional noise tells us about the cell inside. The second IBSE Colloquium was

IBSE Workshop



conducted in June 2018, and the speaker was Dr Anurag Agrawal, Director, CSIR-Institute of Genomics and Integrative Biology, India. Dr Agrawal talked about his interdisciplinary work with maths, biology and medicine. Notably, the colloquia speakers spent quality time interacting with the IBSE students discussing their research and providing suggestions.

IBSE Workshops

Three editions of IBSE Workshop were conducted so far to showcase research activities at IBSE by organising talks by IBSE students and faculty. The workshops were attended by faculty, researchers and students of IIT Madras. These workshops have led to greater awareness of IBSE activities and have initiated a few fruitful advanced discussions on collaborations between IBSE and other IIT Madras faculties.

IBSE Funding

IBSE is grateful to Dr Prakash Arunachalam, Lead Data Scientist, BNY Mellon, USA, for his generous contribution supporting the IBSE and funding IBSE activities through the Office of International and Alumni Relations, IIT Madras. We are also grateful to the Mehta Foundation, USA and Prof Ashok Venkitaraman, Mehta Distinguished Chair for their support.

IBSE Grants

IBSE Research Grant funded two research projects at the interface of biology and engineering. These projects support the preliminary studies to initiate long-term research goals and secure further funding. In “Multi-omics approach to infer potential molecular markers altering disease phenotypes in various tumour stages of adrenocortical carcinoma” project, Dr Indu Gangwar was hired as a postdoctoral fellow and Gaurav Bilolikar as a JRF; and in project titled “Reconstruction and modelling of a *Lactobacillus* co-culture for metabolic engineering of lactic acid”, Dr Maziya Ibrahim was hired as a postdoctoral fellow and Aarthi Ravikrishnan as a JRF. Each award was for ₹8.0 lakhs of which major component was for the training of the postdoctoral fellow.

Publications (2017-18)

1. Bhattacharya P, Raman K, Tangirala AK (2018) A systems-theoretic approach towards designing biological networks for perfect adaptation. *IFAC PapersOnLine* 51: 307.

2. Choobdar S, Ahsen ME, Crawford J, Tomasoni M, Lamparter D, Lin J, Hescott B, Hu X, Mercer J, Natoli T, Narayan R, **The DREAM Module Identification Challenge Consortium**, et al. (2018) Open community challenge reveals molecular network modules with key roles in diseases. *bioRxiv* <https://doi.org/10.1101/265553>.
3. Gopi S, Singh A, Suresh S, Paul S, **Ranu S, Naganathan AN** (2017) Toward a quantitative description of microscopic pathway heterogeneity in protein folding. *PCCP* 19: 20891.
4. Rajasekaran N, Suresh S, Gopi S, **Raman K, Naganathan AN** (2017) A general mechanism for the propagation of mutational effects in proteins. *Biochemistry* 56: 294.
5. Ravikrishnan A, Nasre M, **Raman K** (2018) Enumerating all possible biosynthetic pathways in metabolic networks. *Sci Rep* 8: 9932.
6. Ravikrishnan A, **Raman K** (2018) Systems-level modelling of microbial communities: theory and practice (1st Edition), CRC Press, USA.
7. Sambamoorthy G, **Raman K** (2018) Understanding the evolution of functional redundancy in metabolic networks. *Bioinformatics* 34: i981.
8. Sankar A, **Ranu S, Raman K** (2017) Predicting novel metabolic pathways through subgraph mining. *Bioinformatics* 33: 3955.
9. Sarkar C, Gupta S, Verma RK, **Sinha H, Jalan S** (2018) Longitudinal network theory approaches identify crucial factors affecting sporulation efficiency in yeast. *bioRxiv* <https://doi.org/10.1101/068270>.
10. Yadav A, **Sinha H** (2018) Gene-gene and gene-environment interactions in complex traits in yeast. *Yeast* 35: 403.



New Space

IBSE offices and laboratory are located on the 5th Floor of the new Block-II of the Bhupat and Jyoti Mehta School of Biosciences building. The office has bench spaces for IBSE students and visiting faculty. We are co-located with Robert Bosch Centre for Data Science and Artificial Intelligence (RBCDSAI).

Contact

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