Progress Report of Center of Excellence 2014 – 2015

Funded by Department of Biotechnology Government of India

Center for Computational Biology and Bioinformatics
School of Computational and Integrative Sciences
Jawaharlal Nehru University
New Delhi

The School of Computational and Integrative Sciences (SCIS) is involved in research and teaching programs in areas which are highly interdisciplinary in nature. The major aim of our school is to integrate computational and analytical tools and techniques from different branches of sciences and apply them to get deeper insights into some of the problems which are not hitherto attempted. The school's academic and research programs are currently structured and focused on the core area of Computational and Systems Biology and gradually emphasis is being laid on Complex Systems, Massive Modelling, Simulation and analysis. Department of Biotechnology (Govt. of India) has continued to support our school as **a "Centre of Excellence (COE)"** in Bioinformatics since beginning. Faculties and students are currently pursuing research in diverse fields such as Comparative Genomics, Structural Biology and in silico drug design, Biological Evolution, Biomolecular Simulations, data mining and analysis of large scale data, biophysics, systems biology, robotics, complex systems and artificial intelligence.

SCIS is offering from academic year 2015 ,an integrated **M.Sc.-Ph.D. degree in Computational and Integrative Sciences** with a specialization in either Computational Biology or Complex Systems. The Computational Biology stream will have equivalence to the M.Sc. in Bioinformatics, while the Complex Systems stream will have equivalence to the M.Sc. in Physical Sciences. Additionally, SCIS also offers admission to its Pre-Ph.D. and Direct Ph.D. Programmes in Computational Biology and Bioinformatics. The School has encouraged intake from multiple disciplines into these Programmes - Information Technology, Engineering Sciences, Bioinformatics, the Life Sciences/Biotechnology, the Physical and Chemical Sciences, among others.

An eminent scientist in the field of Econophysics and Sociophysics has been recruited as Professor since last academic year for leading the Program on **"Complex Systems"** in the school in addition to the existing Program "Computational & Systems Biology".

Teaching and research Programs are ably supported by good computational and communication infrastructure consisting of computer clusters with multiprocessor nodes, large-memory nodes and GPUs to facilitate specialized research in the new Building of SCIS.

School of Computational and Integrative Sciences currently offers the following three academic programs for the current year.

(i) Direct admission to Ph.D. program in Computational Biology and Bioinformatics
(ii) Pre-Ph.D./Ph.D. in Computational Biology and Bioinformatics
(iii) M.Sc/Ph.D integrated in Computational and Integrative Sciences Specialization in Computational Biology or Complex Systems

Number of students under Current & earlier Courses offered :

Total No of current Pre-Ph.D and Ph.D Students :	37
Total No of current M.Tech Students	16 1st year
	16 2nd Year
Awarded Ph.D from 2003-2014:	18
No of students awarded M.Tech during 2014:	16
During 2006-2014 M.Tech students passed:	89
Post Graduate Diploma M.Phil (equivalent) in Bioinformatics during 2001-2006:	82

During 2014, Five Students were awarded Ph.D degree and three Ph.D students have submitted their thesis awaiting viva voce examination.

SCIS also has MoU with Queensland University, Australia and BII, Singapore. The student/faculty level exchange has taken place, benefiting the research activity of the School.

Publications during 2013-April to Dec 2014:

1. Palash Nath,Anirban Chakraborti and D. Sanyal "Ab initio calculation of magnetic properties of p-block element doped ZnO", Royal Society of Chemistry Adv.,2014,4, 45598
2. R. Chicheportiche and A. Chakraborti, "Copulas and time series with long-ranged dependences", Phys. Rev. E (2014)89, 042117.
3. A. Chakraborti, D. Challet, A. Chatterjee, M. Marsili, Y.-C. Zhang, B.K. Chakrabarti"Statistical mechanics of competitive resource allocation using agent-based models",, Physics Reports, doi:10.1016/j.physrep. (2015)2014.09.006.
4. R.K. Brojen Singh, Numerical Detection of Stochastic to Deterministic Transition. J. Compt. Nonlinear Dyn. (2014) Doi:10.1115/1.4027441.
5. Kh. Kabita, J. Maibam, B. I. Sharma, R.K.Thapa and R.K. Brojen Singh Density Functional Theory Study of Electronic Structure, Elastic Properties and Phase Transition of Gallium Phosphide (GaP) Adv. Sc. Eng. Med. (2014) 6, 354.
6. BA Ahanger, R. K. Brojen Singh and Z. A. Ansari. Thermal Perturbation in Dye-SensitizedSolar Cell. Mat. Focus (2014), 3,1–5 .
7. Shefeeq. T, N Ahmad, Ravins, R. K. Brojen Singh Diffusional Drug Release from Cylindrical Matrices Into a Finite Medium with Boundary Layer Effect. Adv. Sc. Eng. Med. 6, 948 (2014)
8. Shahnawaz Ali, Md. Z. Malik, Md. J. Alam, R Ishrat and R. K. Brojen Singh. Evolutionary trace analysis of p53 protein: A statistical analysis of conserved aminoacids in p53 protein. Accepted in J. Bioinformatics and Int. Control(2014).
9. Gurumayum Reenaroy Devi , Md. Jahoor Alam, and R.K. Brojen Singh Synchronization in stress p53 network. Mathematical Medicine and Biology(2014) (Accepted)
10. Kh. Kabita, Jameson Maibam, B. Indrajit Sharma, R. K. Brojen Singh and R. K. Thapa. Density functional theory study on pressure induced structural transformation, elastic properties and electronic structure of gallium arsenide (GaAs). Int. J. of Innov. and Appl. Sts. (2014) 8, 382-393
11. Nafis, S., Kalaiarasan, P., Singh, R. B., Husain, M., & Bamezai, R. N. Apoptosis regulatory protein–protein interaction demonstrates hierarchical scale-free fractal network. Briefings in bioinformatics, (2014)doi: 10.1093/bib/bbu036
12. Agarwal, M., Kumar, N., & Vig, L. Non-additive multi-objective robot coalition formation. Expert Systems with Applications, (2014) 41(8), 3736-3747.
13. Amit Srivastava, Rupali Chopra, Shafat Ali, Shweta Agarwal, Lovekesh Vig, and Ramesh Bamezai, "Inferring population structure and relationships using minimal independent markers in Y-chromosome: a hybrid approach of recursive feature selection for hierarchical clustering", Nucleic Acids Research, 2014, 42 (15),
14. Khan, Taushif; Ghosh, Indira. Modularity in protein structures: A study on all alpha proteins. Journal of Biomolecular Structure & Dynamics(2014) (Accepted for publication).
15. Harsh Parikh, Apoorvi Singh, Annangarachari Krishnamachari and Kushal Shah, Computational prediction of origin of replication in bacterial genomes using correlated entropy measure (CEM), BioSystems(2014) (accepted)
16. Mohd Danishuddin, Arbab Khan, Mohammad Faheem, Ponnusamy Kalaiarasan, Mohd Hassan Baig, Naidu Subbarao and Asad U. Khan, "Structure-based screening of inhibitors against KPC-2: designing potential drug candidates against multidrug-resistant bacteria", Journal of Biomolecular Structure and Dynamics, (2014), Vol 32, 5, 741-750
17. Kamaldeep Gill, Lokesh Nigam, Ratnakar Singh,Suresh Kumar, Naidu Subbarao,Dhyam Singh

Chauhan, Sharmistha Dey. The Rational Design of Specific Peptide Inhibitor against p38α MAPK at Allosteric-Site: A Therapeutic Modality for HNSCC(2014). PlosOne (2014) 9 (7), e101525
18. Yachana Jha, Gaurav Sablok, Naidu Subbarao, Raja Sudhakar, M. H. U. Turabe Fazil, R. B. Subramanian, Andrea Squartini and Sunil Kumar Bacterial-induced expression of RAB18 protein in Orzya sativa salinity stress and insights into molecular interaction with GTP ligand. Journal of Molecular Recognition (2014) 27 (9), 521-527
19. Mohd H Baig; D Raja Sudhakar; Ponnusamy Kalaiarasan; Gulshan Wadhawa; Naidu Subbarao; Mohtashim Lohani; Asad U Khan "Effect of inhibitor resistant S130G mutant on physico-chemical properties of SHV type beta-lactamase" . PLOSOne(2014),9(12), e112456
20. Ponnusamy Kalaiarasan, Subarao Naidu, Rameshwar NK Bamezai, Molecular simulation of Tyr105 phosphorylated Pyruvate kinase M2 to understand its Structure and Dynamics. in Journal of Molecular Modeling(2014),20,9,1-12
21. Amit Kumar, Nidhi Agarwal, Lalit Pant, Jay Prakash Singh, Indira Ghosh, Naidu Subbarao; PfalDB: An Integrated Drug Targets and Chemical Database for Plasmodium falciparum. Current Drug Targets(2014),15,12,1089-1093
22. Vijayan Ramachandran, Naidu Subbarao, Manoharan Natesan Homology modeling of LAMMER kinase of *Plasmodium falciparum* and to identify the interaction of crtical resdiues involved in binding of ATP by Molecular docking simulation study, International Journal of Advanced Life Sciences(2014),7,2,311-320.
23. Sinha, S., & Lynn, A. M.. HMM-ModE: implementation, benchmarking and validation with HMMER3. BMC research notes, (2014)7(1), 483.
24. Qayum, A., Lynn, A. M., & Arya, R. Traditional Knowledge System Based GIS Mapping of Antimalarial Plants: Spatial Distribution Analysis. Journal of Geographic Information System, (2014),6(05), 478.
25. P Narang, S Khan, AJ Hemrom, AM Lynn MetaNET-a web-accessible interactive platform for biological metabolic network analysis. BMC Systems Biology(2014) 8 (1), 130.
26. S Singh, U Bajpai, AM Lynn Structure based virtual screening to identify inhibitors against MurE Enzyme of Mycobacterium tuberculosis using AutoDock Vina, Bioinformation(2014) 10 (11), 697
27. Kumari, R., Kumar, R., Consortium, O. S. D. D., & Lynn, A. M. g_mmpbsa-A GROMACS tool for high-throughput MM-PBSA calculations. Journal of chemical information and modeling (2014)54 (7), pp 1951–1962.
28. Meher, B. R., Kumar, M. V. S., & Bandyopadhyay, P.. Interchain hydrophobic clustering promotes rigidity in HIV-1 protease flap dynamics: new insights from Molecular Dynamics. Journal of Biomolecular Structure and Dynamics, (2014)32(6), 899-915.
29. Hasnain, S., McClendon, C. L., Hsu, M. T., Jacobson, M. P., & Bandyopadhyay, P.. A New Coarse-Grained Model for E. coli Cytoplasm: Accurate Calculation of the Diffusion Coefficient of Proteins and Observation of Anomalous Diffusion. PloS one, (2014)9(9), e106466.
30. Sahu, N., Gadre, S. R., Rakshit, A., Bandyopadhyay, P., Miliordos, E., & Xantheas, S. S.. Low energy isomers of (H2O) 25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. The Journal of chemical physics, (2014),141(16), 164304.
31. Singh, P., Sarkar, S. K., & Bandyopadhyay, P. Wang-Landau density of states based study of the folding-unfolding transition in the mini-protein Trp-cage (TC5b). The Journal of chemical physics, (2014)141(1), 015103.
32. Hasnain, S., Jacobson, M. P., & Bandyopadhyay, P.. A comparative Brownian dynamics investigation between small linear and circular DNA: Scaling of diffusion coefficient with size and topology of DNA. Chemical Physics Letters, (2014), 591, 253-258.
33. Jean-Numa Gillet, "Ultrafast molecular dynamics of biofuel extraction for microalgae and bacteria milking: blocking membrane folding pathways to damaged lipid-bilayer conformations with

nanomicelles," in Journal of Biomolecular Structure and Dynamics, Published online: April, 15, 2014, DOI: 10.1080/07391102.2014.907544

Book Chapters/Proceedings

1. MJ Alam, V Singh, RK Brojen Singh. Switching Mechanism in the p53 Regulatory Network Systems and Synthetic Biology (Book Chapter) (2014**)**
2. "Physicists' Approaches to a Few Economic Problems", Anirban Chakraborti, Yoshi Fujiwara, Asim Ghosh, Jun-ichi Inoue and Sitabhra Sinha, in Eds. F. Abergel, H. Aoyama, B. K. Chakrabarti, A. Chakraborti and A. Ghosh, Econophysics and Data Driven Modelling of Market Dynamics (Springer, Milan, 2015)
3. "Maximizing a Psychological Uplift in Love Dynamics", M. Banerjee, A. Chakraborti and J. Inoue, in Eds. R. Lopez-Ruiz, D. Fournier-Prunaret, Y. Nishio, C. Gracio, Nonlinear Maps and their Applications, Springer Proceedings in Mathematics & Statistics (Springer International Publishing, Switzerland, 2015).
4. "Kinetic Exchange Models in Economics and Sociology", S. Goswami and A. Chakraborti, in Eds. R. Lopez- Ruiz, D. Fournier-Prunaret, Y. Nishio, C. Gracio, Nonlinear Maps and their Applications, Springer Proceedings in Mathematics & Statistics (Springer International Publishing, Switzerland, 2015).

JNU DBT –COE was selected for 1st prize during 2011-12 and 3nd Prize during 2012-13 for Publication amongst DBT –COE centers.

Workshop/Conferences during 2014

Indo US Conference and Workshop on Synthetic and Systems Biology" at JNU, New Delhi Nov 9-12, 2014: http://ccbb.jnu.ac.in/IUSSB/

Indo-US Bilateral Conference cum Workshop on "Big Data Analysis and Translation in Disease Biology" at JNU, New Delhi January 18-22 2015 : http://ccbb.jnu.ac.in/IUBDDJan2015/register.php

Research Projects (active):

- DST project on "Development and application of new computational techniques to understand macromolecular properties in realistic cellular environment.". PI: Dr.Pradipta Bandhyopadhyay, 2014-2017.
- DBT project on "Computational Core for Plant Metabolomics" Prof Indira Ghosh with IIIT, Hyderabad, 2011-2015.
- DBT Builder Project, Coordinator: Prof R.Bhat, SBT, JNU (SLS, SCMM and SBT and SCIS faculty of JNU) 2012-2017.
- DST Fast Track for Young Scientist, Automaticity in Robot motor skill learning, Dr Lovekesh Vig, 2013-2016.
- DST project, stochastic synchronization: Complexity in signal processing in interacting system. Role of noise and application ,Brojen Singh, 2013-2016
- CSIR Project Understanding Complex dynamics and information proceeding in Brain Network, Brojen Singh,2013-2016.

The Thesis titles of Ph.D Students (degree awarded) during 2014 :

Name	Ph.D Thesis Title	Supervisor
Dr. Om Prakash	Maximum common substructure based in silico approach for lead and target identification	Prof. Indira Ghosh
Ms. Payal Singh	Sequence and structure based computational study of RNA's	Dr. Pradipta Bandhopadhyay/ Dr Supritam Sengupta
Dr. Sabrashish Das	Comparative analysis and study of ,mutations in Bacterial genomes	Prof. Alok Bhattacharya
Dr Vinekar Rithvik Shamrao	Molecular Dynamics study of functional Oligomers	Prof Indira Ghosh
Mr Amit Kumar	In Silico Profiling of Enzymes Active Site for Specificity and Selectivity: A case Study of Plasmodium falciparum	Prof Indira Ghosh
Mr Rajeev Mishra	Structual Bioinformatics Study of GTPases Lacking the Catalytic Glutamine	Dr Andrew M. Lynn/Dr Balaji Prakash(IIT Kanpur)

The Thesis titles of Ph.D Students (Thesis submitted) during 2014 :

Student	Thesis Title	Supervisor
Ms. Reema Singh	Development and Application of Data Management and Protocols for High Throughput Data Analysis	Dr. Andrew M. Lynn
Ashutosh Viswa bandhu	Origin and evolution of Geneic Code: An Insilico study	Dr Supritam Sengupta/Dr Devapriya Choudhary
Anmol Henroom	Cyberinfrastructure for the Biological Sciences	Dr Andrew Lynn

The Thesis titles of M.Tech Students (degree awarded) during 2014

S.No.	Name of the Student	M.Tech Thesis Tittle	Supervisor
1	Mr. Ankit verma	Deep Convolutional Networks for Image Recognition.	Dr. Lovekesh vig.
2	Mr. Baiateilang Diengngan	Molecular Dynamics simulations to understand the effect of salt on the stability and dynamics of a protein-DNA complex.	Dr. Pradipta Bandyopadhyay
3	Mr. Bhaskar Prasad	Digital Siganl Processing (DSP) based power spectral methods to study the exon-intron structures of few selected genes.	Dr. A. Krishnamachari
4	Mr. Kashif Nawaz	Assembly, Annotation and differential expression analysis from RNA-seq data using Tophat/Cufflinks: Application to Cancer and Rice genome samples.	Dr. Andrew M. Lynn
5	Mr. Mayank Gupta	Development and Application of annotation pipeline for metabolome mapping in Genome sequences.	Dr. Andrew M. Lynn
6	Ms. Neha Anand	Application of Baysian Network in analysis of Biological systems.	Prof. Indira Ghosh
7	Mr. Niranjan Kumar	Virtual Screening of antimalarial (Bioactive) compounds against Prioritized *Plasmodium falciparum* Drug Targets.	Dr. Naidu Subbarao
8	Mr. Rakesh Srivastava	Analytical study of spherical multilayer solvent system electrostatics and its application to encapsidation of simple virus model.	Dr. Pradipta Bandyopadhyay
9	Mr. Ravishaker Soni	Recurrent Neural Networks for Temporal Sesquential Prediction.	Dr. Lovekesh Vig.
10	Mr. Saurabh Kumar Sharma	The synchronization of genetic oscillators induced by miRNA.	Dr. R. K. Brojen Singh
11	Mr. Shailendra Kumar Singh	Digital Signal Processing (DSP) based filters for studying functional sides: a case study of CpG islands.	Dr. A. Krishnamachari
12	Mr. Shakti Nath Singh	Role of time delay in stochatic systems.	Dr. R. K. Brojen Singh
13	Mr. Sintoo Kumar	Digital Signal Processing (DSP) based analysis of Genomes: a computational study through MPI implementation	Dr. A. Krishnamachari
14	Mr. Tarun Kumar Gupta	Deep Autoencoders for non-linear dimentionality reduction.	Dr. Lovekesh Vig.
15	Mr. Vipin Ranga	Microarray Meta-Analysis workflow development and application in the identification of important marker genes in primary Sjogeren's syndrome.	Dr. Andrew M. Lynn
16	Mr. Yogendra Kumar Bhaskar	Assembly, Annotation and differential expression anlysis from RNA-Seq data using Trinty: Application to the de-novo sequence of the Indian Pitcher plant.	Dr. Andrew M. Lynn

List of Summer Trainee 2014 :

Name	Affiliation	Supervisor
Sonali Mishra Sonalimishra013@gmail.com	IIIT, allhabad	Dr.Naidu Subbarao
Deepa justdeepahbti@gmail.com	IIIT Allhabad	Dr.Naidu Subbarao
Sanjeet Maisnam sanjeet.maisnam3@gmail.com	NISER Kolkota	Dr.R.K.Brojen
Deboshmita Sen debo.iuac@gmail.com	SV College, Delhi University	Dr.Narendra Sahni
Lokesh Sharma lokeshsam555@gmail.com	JUIT, Solan	Dr.A.K Chari
Vikaran Singh Thakur nit159357@gmail.com	JUIT, Solan	Prof RNK Bamezai
Nimisha nimisha.mishra17@gmail.com	OUAT, Bhuvaneswar	Dr. Naidu SubbaRao
Kishor Kumar Kumawat kumawatkishor12@gmail.com	IISER, Calcutta	Dr.R.K.Brojen

List of Long Term Trainees 2014

S.No	Name	Affiliation	supervisor
1	Ms Yasmin Fatima	Jamia Millia Islmaia University	Brojen Singh
2	Ms Samar Fatma	Jamia Millia Islmaia University	Prof RNK Bamezai
3	Antara Mazumdar	Jamia Millia Islmaia University	Naidu Subbarao
4	Ms Garima Singh	Jamia Hamdard University, N Delhi	Prof Indira Ghosh
5	Irfan Rasool Bhat	Jamia Millia Islmaia University	Prof RNK Bamezai
6	Mohd Waseem	Jamia Millia Islmaia University	Naidu Subbarao

Future Plan

- Eight faculty positions in SCIS are to be recruited soon.
- Two G.N.Ramachandran Fellowships and few technical positions will be filled up.
- All the faculty, staff and students moved to New SCIS building in 2014 and requirement of Project facilities to be procured.
- M.Sc/PhD Integrated program in Computational and Integrative Sciences with specialization Computational Biology and Complex Systems will be offered from the forthcoming academic year 2015.
- Improving Infrastructure in High Performance computing Facility in New Building

Prof Indira Ghosh **Dr. N. Subba Rao**

Coordinator, **CO-Coordinator,**

DBT-Centre of Excellence in Bioinformatics

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