Computational Biology and Bioengineering

An AcSIR – Engineering Science course of study at CSIR –NCL

Objective

This PhD program will be an integrative and inter-disciplinary program aimed at understanding and engineering biology using mathematical and computational techniques. A graduate of this program is expected to become familiar with and apply a diverse set of theoretical and computational techniques as needed for addressing contemporary research in biology. Successful graduates will receive a PhD degree in Engineering Sciences from AcSIR.

Why CSIR-NCL

CSIR-NCL is ideally suited to offer this program for the following reasons. Many scientists in CSIR-NCL, with diverse background and expertise, are actively carrying out research in the broad area of computational biology addressing topics ranging in scale from single molecules to population/ecosystems. Techniques used include molecular modeling, machine learning, reaction engineering, constraints-based analysis, bioinformatics, chemoinformatics, and dynamical systems. This puts CSIR-NCL in a unique position to offer truly interdisciplinary training, with students being taught by engineers, mathematicians, chemists, and biologists. In addition to a strong biological sciences program at CSIR-NCL, active external collaborations already exist with groups in premier research institutes like IISER Pune, NCCS, CSIR-IGIB and University of Pune. Students of this program will greatly benefit from this collaborative network through interactions with researchers from these institutes and by having access to their facilities. Moreover, CSIR-NCL has a state of the art computational infrastructure, including computer clusters, which is fully capable of catering to the needs of the students enrolling into this program.

Participating Faculty (Division wise)

Chemical Engineering and Process Development: Anu Raghunathan, BD Kulkarni, Chetan Gadgil, Leelavati Narlikar, Mugdha Gadgil, Ram Rup Sarkar, Ravi Kumar, Sanjeev Tambe
Biochemical Sciences: C. G. Suresh, Dhanasekaran Shanmugam, Kiran Kulkarni, , Narendra Kadoo, Sureshkumar Ramasamy,
Physical Chemistry: Debashree Ghosh, Durba Sengupta, Kumar Vanka, Neelanjana Sengupta, Suman Chakrabarty
Digital Information Resource Center: M. Karthikeyan

Admission-criteria

Candidate must have a 4-year undergraduate degree, or Masters degree in relevant branches of science, engineering or pharmacy, as per AcSIR rules. He/she will be expected to have an undergraduate-level training in either numerical/ mathematical/ statistical sciences/engineering; or in biology/biophysics. Exact details are available on the NCL or AcSIR admissions site. For the August 2015 session, students are expected to have a national-level fellowship such as CSIR/UGC/BINC/DBT/ICMR/INSPIRE etc that is tenable at NCL on the date of the interview.

Evaluations

1. Selection interviews will be conducted by a separate committee comprising of computational and experimental biologists. The interview will test basic analytical and logical skills of the candidate. Knowledge in one of Biology and Computation/ Mathematics will be a prerequisite.
2. DACs will include one scientist from an unrelated area other than subject experts.
3. Qualifier/comprehensive exams will be conducted by a common panel, which will test the candidate's understanding of the subject of his/her undergraduate degree and the field that he/she has decided to focus on.

Planned interactions outside CSIR-NCL

Given the close collaborations between CSIR-NCL and industry, it is expected that the students will gain exposure to industrially relevant problems and be able to participate in such programs. It is expected that some students will be funded by the relevant industries.

Coursework[1]

Core courses[2]

1. Fundamentals of Biology (3 credits)
Course Objective
To review biology fundamentals, provide an introduction to students with a non-biology background. Course will focus on core concepts and a quantitative view of biology.

2. Mathematical Fundamentals (3 credits)
Course Objective
To review mathematical fundamentals, teach common mathematics prerequisites of other courses, and to impart perspective on modeling and simulation.

3. Numerical Methods and Programming (3 credits)
Course Objective
To introduce the numerical methods used for computational modeling of biological processes. Students will develop the ability to analyze and implement an appropriate algorithm for different numerical techniques using a modern programming language.

4. Statistical Analysis (3 credits)
Course Objective
To ensure students develop competence in statistical analysis required for their research.

Optional courses

Several optional courses ranging from sequence analysis, biomolecular structure and dynamics to intracellular modeling and bioreactor analysis will be offered. Also included in these are mini-projects where students can undertake a semester-long project individually or as part of a team.

[1] AcSIR-wide compulsory courses such as the 4-level courses are not specifically listed, but are of course also required for students in this program

[2] These four courses are compulsory; credits can also be earned via clearing a 'challenge' test at the beginning of the semester, or waived if the course has been completed as part of the requirements for another AcSIR program (such as MS-Res)

Faculty Profiles

Name/Contact details	Education and Experience	Research Interests
Dr. Anu Raghunathan Scientist, CSIR-NCL Phone: 020-25903067 Email: anu.raghunathan@ncl.res.in 	• Faculty (Research), Mount Sinai (Medicine), NY • Post-doctoral Fellow, Bioengineering, University of California San Diego • Post-Doctoral Fellow, Microbiology and Cell Science, Univ of Florida • Ph.D., Chemical Engineering, IIT Bombay • M.S., Anal. & Med. Chem, SNDT, Mumbai	• Metabolic network reconstruction and constraints based analysis of biological systems • Microbial strain design for use of renewable resources, systems biology and molecular adaptation to produce and improve yields. • Drug Target Discovery: Systemic approaches (computational and experimental) to study metabolism in pathogenesis to discover novel drug targets.
Dr B. D. Kulkarni Scientist, CSIR-NCL Phone: 020-25902150 Email: bd.kulkarni@ncl.res.in 	• PhD, Chemical Engineering, University of Pune • M. Tech, Chemical Engineering, LIT, Nagpur • B Tech Chemical Engineering, LIT Nagpur	• Chemical reaction engineering • Mathematical modeling • Optimization and control • Process design • AI in bioprocess monitoring and control • Bio-inspired optimization algorithms
Dr C. G. Suresh Scientist, CSIR-NCL Phone:020-25902236 Email: cg.suresh@ncl.res.in 	• Research Associate, Molecular Biophysics Unit, IISc. • PhD, Molecular Biophysics Unit, IISc	• Structural Biology • Biomolecular Crystallography and conformational analysis • Molecular modelling and Bioinformatics • Genetics and Evolution • Ntn hydrolases, plant lectins and protease inhibitors • Mitochondrial proteins
Dr Chetan Gadgil Scientist, CSIR-NCL Phone: 020-25902163 Email: cj.gadgil@ncl.res.in 	• Investigator, GlaxoSmithKline, USA • Postdoctoral research associate, School of Mathematics, U. Minnesota • Ph.D., Chemical Eng, Univ. of Minnesota, USA • M Tech, Chemical Engineering, IIT Bombay • B. Chem. Eng. ICT (formerly UDCT), Mumbai.	• Mechanistic models of biological systems: regulatory networks, other cellular processes • Modeling/Simulation of patterning in biology • Stochastic models for (bio) chemical reactions • Modeling drug delivery and distribution kinetics

Dr Debashree Ghosh Scientist, CSIR-NCL Phone:020-25903052 Email: debashree.ghosh@ncl.res.in 	• Post Doctoral Research Fellow, University of Southern California, USA • PhD, Cornell University, Ithaca, NY	• Electronic structure theory
Dr Dhanasekaran Shanmugam Scientist, NCL Phone: 020-25902719 Email: d.shanmugam@ncl.res.in 	• Postdoctoral fellow, Department of Biology, U. Pennsylvania, Philadelphia, USA (2004-2011) • Ph.D., Biochemistry Department, IISc, Bangalore, (1997-2003) • M.Sc. Medical Biochemistry, Pondicherry University, (1994-1997) • B.Sc. in Biochemistry, Bharathiyar University (1991-1994)	• Biochemistry and molecular parasitology; • MS and NMR metabolomics • Anti-malarial screening and mechanism of action studies • Eukaryotic parasite genomics.
Dr Durba Sengupta Ramalingaswami Fellow Phone: 020-25902408 Email: d.sengupta@ncl.res.in 	• PostDoctoral Research Associate (2006-2011), University of Groningen, Netherlands • PhD (Biosciences) 2005, University of Heidelberg, Germany • Msc (Bio Chem) IIT Powai, Mumbai 2001 • B.Sc., (Chemistry) Univ. of Delhi, 1999	• Self Organisation and Self Assembly in cellular membranes • Multi-scale simulation approaches from the atomistic to mesoscopic length scales
Dr M. Karthikeyan Scientist, CSIR-NCL Phone: 020-25902483 Email: m.karthikeyan@ncl.res.in 	• Post Doctoral Research Fellow (Prof Alex Tropsha, University of North Carolina, USA)2003-04, 2007-08 • MSc Comp. Science, Anna University • PhD (Chemistry), Pune University (NCL) • BSc and MSc Chemistry, Pondicherry University	• Organic Chemistry • Molecular Informatics • Chemoinformatics, • Bioinformatics & Computational Chemistry • Drug Design and Virtual Screening • Computational Industrial Risk Assessments

Dr Kiran Kulkarni Scientist, CSIR-NCL Phaone: 020-25902720 Email: ka.kulkarni@ncl.res.in 	• Post-doctoral Fellow, Institute of Cancer Research, London. • Application Scientist, JNCASR, Bangalore. • Ph.D. IISC (Structural Biology) • M.Sc., Karnatak University, Dharwad (Solid State Physics) • B.Sc. Karnatak University, Dharwad (Electronics)	• Structural Biology; Cellular Signaling Networks; Cancer Biology; Method Development in X-ray Crystallography and Cryo Electron Microscopy.
Dr Kumar Vanka Scientist, CSIR-NCL Phone:020-25902083 Email: k.vanka@ncl.res.in 	• Postdoctoral fellow, (CEBC), Kansas University • Ph.D., Chemistry, University of Calgary, Canada. • M.Sc., Chemistry, University of Calgary. • BSc. Chemistry, Indian Institute of Technology, Khargapur.	• Chemical Storage of Hydrogen • Investigation of the Reaction Mechanism of Transition Metal Complexes • Accelerated Stochastic Simulations
Dr Leelavati Narlikar Scientist, CSIR-NCL Phone:020-25903076 Email: l.narlikar@ncl.res.in 	• Research Associate, Centre for Modeling and Simulation, Pune University • Postdoctoral Fellow, National Institutes of Health, MD, USA • PhD, Computer Science, Duke University, 2008 • BE, Computer Engineering, Pune University, 2002	• Machine learning: Supervised and unsupervised learning from large scale data; Bayesian modeling; Statistical optimization algorithms • Computational biology: Identifying gene regulatory elements; Mapping networks of transcriptional regulation; Understanding the role of epigenetics in regulation
Dr Mugdha Gadgil Scientist, CSIR-NCL Phone:020-25902433 Email: mc.gadgil@ncl.res.in 	• Scientist, Invitrogen Corporation, MD, USA • Postdoctoral research associate, University of Minnesota, MN, USA • Ph.D., Chemical Eng, University of Minnesota, MN, USA, 2004. • B. Chem. Eng. ICT (formerly UDCT), Mumbai, 1999.	• Bioinformatics: developing methods for analysis of DNA microarray data • Bioprocess engineering for cell culture processes

Dr Narendra Kadoo Scientist, CSIR-NCL Phone: 020-25902724 Email: ny.kadoo@ncl.res.in 	• Visiting Scientist, CSIRO Plant Industry, Brisbane, Australia • Ph.D. (Genetics), Indian Agricultural Research Institute, New Delhi • M.Sc. (Genetics), IARI, New Delhi • B.Sc. (Agriculture), Dr. PDKV, Akola, Maharashtra • Advanced Diploma in Web Enabled Database Technologies from C-DAC, Pune	• Plant-pathogen interactions at molecular and biochemical levels • Bioinformatics analysis of gene families • Comparative genomics • DNA barcoding and genetic diversity analysis
Dr Neelanjana Sengupta Scientist, CSIR-NCL Phone: 020-25902087 Email: n.sengupta@ncl.res.in 	• PhD, Physical Chemistry, Univ. of California, Irvine, 2008 • M.S, Chemical & Materials Physics, Univ. of California, Irvine, 2007 • M.Sc., Physics, Univ. of Burdwan, 2000 • B.Sc., Physics, Univ. of Burdwan, 1998	• Understanding amyloid formation and protein aggregation diseases • Protein translocation through membranes • Solvent dynamical coupling in biomolecules • Transport and signaling phenomena in biomolecular confinement
Dr Ram Rup Sarkar Scientist, CSIR-NCL Phone:020-25903040 Email: rr.sarkar@ncl.res.in 	• Post-Doctoral Fellow Institute for Environ. Systems Research, University of Osnabrueck, Germany, 2004-2005 • Ph.D. (Science), Indian Statistical Institute & Jadavpur University, Kolkata, 2004. • MSc., (Appl. Math), University of Calcutta, Kolkata, 1999. • Scientist, CSIR-CCMB, Hyderabad (2005-2012)	• Study of Biochemical reaction pathways (Gene regulatory, Metabolic and Signaling); Cellular interactions. • System Biology of Cancer: Modeling signaling and metabolic pathways in Immune and Cancer cells; Deterministic and Stochastic modeling of tumor-immune interactions. • Infectious Diseases: Mathematical and Statistical modeling, Time Series Analysis; Study of spatio-temporal spreads.
Dr. V. Ravi Kumar Scientist, CSIR-NCL Phone: 020-25902161 Email: v.ravikumar@ncl.res.in 	• Postdoctoral Research Associate, (1984 -1986), Department of Chemical Engineering, Texas A&M University, TX, USA • Ph.D., Chemical Engg. Division, National Chemical Laboratory & University of Pune, India • M.Sc., Chem. Dept., Bangalore University	• Nonlinear dynamics, chaos and turbulence • Chemical reaction engineering • Analysis of networks • Parameter estimation, optimization and control • Noise reduction in nonstationary data • Classification, pattern formation and feature extraction from space-time data

Dr. Sanjeev Tambe Scientist, CSIR-NCL Phone: 020-25902156 Email: ss.tambe@ncl.res.in 	• Visiting Scientist, Department of Chem. Eng., University of Louisville • Research Associate at Department of Geology, University of Louisville, Louisville, KY, USA. • Ph.D., (Physical Chemistry) CSIR-NCL & Univ. of Bombay • M. Sc. (Analytical Chemistry) Department of Chemistry, University of Bombay	• Design, development and application of Artificial Intelligence and machine learning formalisms to chemical & biological systems. • Modeling and optimization of reactions/reactors; control and analysis of nonlinear systems • Chemical reactor/reaction modeling via phenomenological, stochastic, cellular automata, and Monte Carlo approaches • Applications of fractal theory and multi-variate statistics.
Dr Suman Chakarbarty Ramanujan Fellow, CSIR-NCL Phone: 91-20-25903053 Email: s.chakrabarty@ncl.res.in 	• Post Doctoral Research Fellow, University of Southern California, USA • PhD, Solid State and Structural Chemistry Unit, IISc	• Hydrophobic effects, and phase transition related phenomena in soft-condensed matter systems • QM/MM study of chemical reactions in solution and enzyme catalysis • Protein electrostatics: pKa calculation, solvation energy, binding energy • Biomimetic design of functional materials: with focus on ion channels, aquaporins etc.
Dr Sureshkumar Ramasamy Ramanujan Fellow, Phone: 020-25902797 E.mail: s.ramasamy@ncl.res.in 	• Staff Scientist: California Institute of Technology (Caltech), Pasadena, CA. • Ph.D in Structural Biology, NCL, Pune • M.Sc (Agri) Biotechnology, University of Agricultural Science, Bangalore • B.Sc (Agri) Tamil Nadu Agricultural University, Coimbatore, India	• Structural Biology and Bioinformatics; • Protein translocation pathway and cell signaling.