



ANNUAL PROGRESS REPORT: 2004 - 2005

BioInformatics Research Centre (BIRC)
Nanyang Technological University, Singapore

Compiled By:
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Executive Officer

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I. INTRODUCTION

The BioInformatics Research Centre (BIRC) which was established on March 1, 2002, is the focus of the education, research and development, and human-resource training in bioinformatics at NTU. BIRC is an inter-school research centre hosted by the School of Computer Engineering (SCE). Currently 25 staff members from SCE, SBS, NIE, MAE, and EEE are affiliated and based their research projects at BIRC. It has 8 full-time researchers and 19 Ph.D. students.

Bioinformatics is the field of analyzing biological data, such as sequences, expressions, phenotypes, images, and literature, to discover biological knowledge leading to discover novel drugs and therapeutics. The mission of BIRC is to provide the interdisciplinary environment and training for students and researchers to engage in leading and cutting edge research in bioinformatics at NTU, and thereby become a part of the life sciences workforce in Singapore and elsewhere. BIRC brings together scientists and engineers, who are interested in bioinformatics modeling and computation, and fosters cross-disciplinary interactions among different schools to perform advanced research in bioinformatics. It also facilitates the teaching and research projects of the MSc. (Bioinformatics) offered by SCE.

Mission: The BioInformatics Research Centre (BIRC) has a mission to provide interdisciplinary environment and training for students and researchers to engage in leading and cutting edge research in bioinformatics in NTU, and thereby become a part of the life sciences workforce in Singapore and elsewhere.

Vision: The Centre's vision is to dedicate itself to the advancement of bioinformatics through education, research, and scientific breakthroughs, leading to discoveries of new medical drugs and therapies.

II. RESEARCH INTERESTS

The interests of staff in the center are distributed across its research areas:

<p>GENOMICS Computational genomics, gene structure prediction, comparative genomics, phylogenetic studies, gene expression analysis</p>	<p>A/P Jagath Rajapakse (SCE) A/P Lin Feng (SCE) Adj Prof Wong Limsoon (SCE) A/P Tan Eng Chong (SCE) Asst/P Jagdish Patra (SCE) Asst/P Vivekanand Gopalkrishnan (SCE) Asst/P Li Jinming (SBS) Asst/P Huang Guangbin (EEE) A/P Wang Lipo (EEE) A/P Shu Jianjun (MAE)</p>
<p>STRUCTURAL GENOMICS AND PROTEOMICS Protein structure prediction, protein-protein interactions, protein classification, modeling, and docking, mass spectroscopy.</p>	<p>A/P Jagath Rajapakse (SCE) A/P Kwoh Chee Keong (SCE) A/P Lin Feng (SCE) A/P Narendra Chaudhari (SCE) Adj A/P Kolatkar Prasanna (SCE) Adj A/P Ng See Kiong (SCE) Adj Prof Wong Limsoon (SCE) Asst/P Vivekanand Gopalkrishnan (SCE) Prof Lars Nordenskiold (SBS) Prof Salil K. Bose (SBS) A/P Chia Tet Fatt (NIE) A/P Wang Lipo (EEE) A/P Shu Jianjun (MAE) A/P Cai Yiyu (MAE)</p>
<p>SYSTEMS BIOLOGY Tissue systems biology, neural systems biology</p>	<p>Prof Dhanjoo Ghista (MAE) A/P Liao Kin (SCBE) A/P Jagath Rajapakse (SCE) A/P Kwoh Chee Keong (SCE)</p>
<p>BIOLOGICAL DATABASES, MINING, AND VISUALIZATION Biological data integration, storage, and query processing, 3-D visualization.</p>	<p>Prof Duch Wlodzislaw (SCE) A/P Lin Feng (SCE) Adj Prof Wong Limsoon (SCE) Asst/P Sourav Bhowmick (SCE) Asst P Fong Cheuk Ming (SCE) Asst/P Vivekanand Gopalkrishnan (SCE) A/P Wang Lipo (EEE) A/P Cai Yiyu (MAE)</p>
<p>FUNCTIONAL AND CELLULAR IMAGE INFORMATICS Functional brain imaging, cellular imaging, microarray and electrophoresis image analysis, bioimaging informatics</p>	<p>A/P Jagath Rajapakse (SCE) A/P Lin Feng (SCE) A/P Tan Eng Chong (SCE) Asst Prof. Vitali Zagorodnov (SCE) Asst Prof Jagdish Patra (SCE) A/P Wang Lipo (MAE)</p>
<p>DRUG DISCOVERY AND TRIAL DESIGN Immunoinformatics, modeling human immune system</p>	<p>Adj Prof Wong Limsoon (SCE) Adj A/P Valdimir Brusic (SCE) Adj A/P Prasanna Kolatkar (SCE) Prof Dhanjoo Ghista (MAE) A/P Cai Yiyu (MAE)</p>
<p>COMPUTING SYSTEMS FOR BIOINFORMATICS Parallel algorithms and architectures for bioinformatics, grid computing, embedded systems for bioinformatics</p>	<p>A/P Lin Feng (SCE) Asst/P Bertil Schmidt (SCE) Asst/P Ong Yew Soon (SCE)</p>

III. RESEARCH FUNDING

The research funding for the centre comprises of the following:

List of current research projects					
S/No	Project Title	Source Of Funding	Principle Investigators/ Collaborators	Amount of Funding S (\$)	Duration (Date)
01	Bioinformatics	NTU/ Compaq	Dean, SCE	\$1,500,000	2002 - 2006
02	Bio-visualisation	A*Star	A/P Cai Yiyu	\$748,000	2003-2006
03	Elucidation of Expression Profiles of Genes in Alpha-fetoprotein Positive and Alpha-fetoprotein Negative Hepatocellular Carcinoma by cDNA Microarray Analysis	BMRC & NMRC	A/P Lin Feng (collaborator)	\$113,000	2004
04	Design and Simulation of Artificial Bone Implantation	MOE & ARF	A/P Lin Feng	\$17,402	2001-2004
05	Analysis of functional brain images	RGM11/03	A/P Jagath Rajapakse	\$140,000	Oct 2003 – Oct 2006
06	Neural systems modeling using functional MRI	MOE & A*STAR	A/P Jagath Rajapakse	\$658,320	Oct 2002 – May 2006
07	Advanced Analysis of Cellular Images	SMA2-CSB program	A/P Jagath Rajapakse/ Prof. Roy E. Welsh, MIT, USA	\$223,000	Aug 2005 – Aug 2008
08	Grid-based comparative genomic pipeline for detecting conserved non-coding functional regions	A*Star BMRC Grant through National Grid Office	A/P Jagath C. Rajapakse (PI), Asst. Prof. Miao Chun Yan, Asst. Prof Vivek Gopalkrishnan, A/P Yang Zhonghua	\$143,200	Sept 2005 – Sept 2007
09	Strategic research initiative at Techno Plaza	RGM 4/03	A/P Jagath Rajapakse (Co-PI)	\$150,000	Jul 2003 – Dec 2004
10	Markov Random Field based spatial regularization for fMRI detection	CE – SUG 2/04	Asst Prof Vitali Zagorodnov	\$15,625	Oct 2004 – Oct 2005
11	Smart Laboratory Initiative: The Virtual Lab Dashboard”, Embedded and Hybrid Systems Programme (Main Phase)	Science and Engineering Research Council & A*Star	A/P Ng See Kiong	\$377,000	2003 - 2005

Total Funding: S\$4,058,547

IV. RESEARCH PROJECTS

Title: Neural Systems Biology

Investigators: A/P Jagath C. Rajapakse, Dr. Susanta Mukopadhyay, Dr. Yang Wang, Miss Keren Happuch Fan Fen E.

Collaborators: Dr. Lee Wei Ling, National Neuroscience Institute, Dr. W. Lim, Singapore General Hospital; Dr. Y. Y. Sitoh, National Neuroscience Institute, A/P Susan Rickard Liow, National University of Singapore, Dr. J. J. Chin, Tan Tock Hospital; Dr. Samuel Ng, Mt Elizabeth Hospital; Dr. Frithjof Kruggel, University of Leipzig; Prof J. Hennig, University of Freiburg.

Funding: NTU, MOE, and A*Star, Singapore.

Description:

There have been many successful research efforts in identifying the cognitive function for individual brain areas involved in various cognitive tasks, but the analysis of global effective connectivity have not been investigated thoroughly. In this project, we explore how specialized brain areas interact and how these interactions lead the brain to materialize a certain functional task though brain mapping and gene mapping techniques. This project seeks to find a general framework for modeling interactions among neuronal substrates involved in higher cognitive functions. The main aim is to model neural systems by using probabilistic graphical models from functional MR (fMR) imaging data, in which the interactions among brain regions seen in functional images are expressed in terms of conditional probabilities so that the neural systems and connectivity hypotheses involved in brain diseases such as stroke, Alzheimer's disease, dyslexia, etc. can be studied. The probability densities characterizing graphical models describe complete behavior of a network. Therefore, in theory, graphical model representation renders more information about the brain connectivity. Further, attempts are being taken to separate the neural systems into independent subsystems by using Independent Component Analysis (ICA). We provide experiments done on normals and stroke patients to illustrate how the disconnectivity hypotheses in brain disease could be tested by using the proposed approach.

Title: Analysis of the involvement of Parkinson's Disease (PD) Candidate Genes with a Comparative Genomic Approach

Investigators: A/P Jagath C. Rajapakse, Mr. Gavyn W.L Pang

Description:

Candidate genes of Parkinson's disease include α -synuclein, parkin, ubiquitin C-terminal hydrolase, SPR, TGFA, P450RAI-2 and CP2, which are located in various loci of human. Orthologues to these genes in other species such as chimp, chicken, mouse, rat, fugu and tetraodon provide an opportunity to undergo a comparative analysis of the candidate genes in various species. By conducting the evolutionary study, we attempt to infer how they evolved both structurally and functionally. By analyzing how the genes signals to in the regulatory networks to communicate through various pathways, this project attempts to understand the disease, leading to the discovery of better drugs and treatments; many of the genes involved here have evoked pharmaceutical interest as they have roles in the regulation of peptide hormones. This study may be able to determine PD candidate genes that possess hereditary traits and play significant role in the disease formation.

Title: Molecular Evolution Studies of the Immunity Related Genes from Different Primate Species through Codon Usage Bias Pattern Analysis and Promoter Region Analysis

Investigators: A/P Jagath C. Rajapakse, Dr. Jianmin Ma

Description:

The main purpose of our project is to analyze the codon usage bias patterns of the immunity related molecules such as the MHC, immunoglobulin, and TCR for their classification and to compare their characteristics among different primate species including human beings by performing evolutionary studies. Evolutionary studies of the promoter regions of these genes will also be performed. This project investigates:

1. Codon usage pattern analysis of 1841 HLA sequences, and its application on gene classification using multivariate statistical methods or machine learning methods.
2. Codon usage pattern analysis of 743 MHC sequences from non-human primate (NHP) species, and its application on the molecular evolution studies of the MHC genes using multivariate statistical methods or machine learning methods.
3. Molecular evolution studies through promoter analysis of MHC sequences from different primate species including human beings.

The project will be extended to include the MHC molecules from other available mammal species as well as the immunoglobulin and TCR molecules.

Title: Recognition of Translation Initiation Sites (TIS) and Alternate TIS (ATIS) in eukaryotes

Investigators: Ho Sy Loi, A/P Jagath C. Rajapakse

Collaborators: Dr. Alex V. Kochetov, Institute of Cytology and Genetics, Russian Academy of Sciences, Novosibirsk, Russia

Description:

The failure of translation from mRNA to protein causes the ceasing of subsequent biological processes. At the initiation of translation, a small ribosomal subunit binds at the 5'-end of an mRNA and migrates linearly until the first AUG triplet in an appropriate context is encountered. Under yet unknown circumstances, translation can be initiated at the other AUG(s) sites thereby producing more than one protein from mRNA. A large number of mRNAs contains AUGs within the 5'-untranslated region and/or annotated translation initiation sites in a suboptimal context. It is likely that a portion of ribosomes can initiate translation at downstream AUG and produce additional polypeptides. However, there is an important lack of knowledge on the protein sequences as they are mostly predicted on the base on CDS annotation within cDNA. This project aims to develop a new recognition techniques for translation initiation sites (ATS) and alternative translation initiation sites (ATIS) that could replace wet-lab experiments. We attempt to achieve this by combining Markov chain models, protein-encoding models, and ribosome-scanning models with neural networks. This allows identifying relevant and discriminatory properties of potential sites when insufficient data are available model complex dependencies among the nucleotides. This project will identify features of the mRNA that possibly contribute to its translation at TIS and ATIS sites.

Title: Cancer classification with gene and protein expression data

Investigators: A/P Jagath C. Rajapakse and Dr. Kai-Bo Duan

Collaborators: A/P Francisco Azuaje; Dr. Haiying Wang, University of Ulster Jordantown, North Ireland; Prof. Roy Welsch; Dr. Alex Smaronov, MIT, USA

Description:

This project addresses the problem of cancer classification with expression data collected by microarrays and mass-spectra spectroscopy. Firstly, it develops methods based on SVM-RFE (Support Vector Machine – Recursive Feature Elimination) method to identify relevant genes from gene-expression data and to identify relevant peaks from MS spectroscopic data. We find that SVM-RFE always selects the best peak subset which always has in the top ranked peaks detected by T-statistics. Our finding supports that the selection of a small subset of peaks not only improves the efficiency of the algorithm, but also improves the cancer classification accuracy. The project will further investigate into multi-class and time-series expression data to derive gene regulatory networks that are implicated in different classes of cancer.

Title: Protein Structures and Interactions Prediction

Investigators: Mr. Nguyen Ngoc Minh and A/P Jagath C. Rajapakse

Collaborators: Dr. Shandar Ahmad, Department of Bioscience and Bioinformatics, Kyushu Institute of Technology, Japan; Dr. Jarek Meller, Children's Hospital Research Foundation, Cincinnati University Hospital, USA; Prof. A. Keith Dunker, School of Molecular Biosciences, Washington State University, USA

Description:

The low accuracies of existing approaches for the prediction of three-dimensional (3-D) structures of proteins from their amino-acid sequences have limited the advances in novel drug discovery. Protein-protein interactions play a central role in numerous processes in biological cells and are one of the main focus of the research in this project. We propose Two-Stage Support Vector Machines (TSSVM) and Two-Stage Support Vector Regression (TSSVR) for the prediction of structural properties of amino acid residues, namely, relative solvent accessibilities, protein secondary structure, and solvent accessible surface area elements. The second stage of TSSVM and TSSVR extends the classical SVM and SVR approaches to capture the contextual information among the secondary structural elements or the solvent accessibilities and thereby improves the accuracies of the predictions. We further extend this approach to aid the prediction of the 3-D structure of proteins and protein-protein interactions.

Title: Elucidation of Expression Profiles of Genes in Alpha-fetoprotein Positive and Alpha-fetoprotein Negative Hepatocellular Carcinoma by cDNA Microarray Analysis

Investigator: A/P Lin Feng

Funding: Biomedical Research Council & National Medical Research Council, Joint Research Fund, 2004

Description:

There is little known regarding genetic alterations responsible for specific phenotypes of hepatocellular carcinoma. Currently, genome-wide expression of hundreds of genes can be analysed simultaneously with cDNA microarray technology. This unique technology affords an opportunity to study liver carcinogenesis, which is believed to be a multistep process involving several genetic alterations. The clinical observation is that patients with hepatocellular carcinoma may express alpha-fetoprotein (AFP) in high titres or have normal

titres for AFP. In addition, alpha-fetoprotein has been shown to be useful in prognosticating patients with hepatocellular carcinoma¹⁻⁴. Patients with high AFP titres have been shown to have larger tumours, poorer median survival and more aggressive biological behaviour characterised by multifocality. The intuitive question is that there may be a genetic basis for this observed clinical difference. Hence, our proposed study to elucidate the genetic profile of these two clinical entities of hepatocellular carcinoma may contribute to our understanding of liver carcinogenesis.

Title: Design and Simulation of Artificial Bone Implantation

Investigator: A/P Lin Feng

Funding: Ministry of Education, Academic Research Fund, 2001-2004

Description:

This project is to develop a software system for design and simulation of artificial bone implantation, with the experiments of the physical model fabrication and clinical test. It is an interdisciplinary research project between staff from computer engineering and materials engineering, with the support of clinical staff from Singapore General Hospital (SGH).

A joint project between SGH and the School of Materials Engineering, NTU has successfully used a composite bio-material for artificial bone implantation. The clinical experiments with animals have shown the great potential to apply this material for implantation in human bodies. To realize the potential value of the material, technologies for precise design and fabrication of the implants should be developed. Tissue growth and other relevant processes in the implantation should also be studied. The proposed software system is to provide these functions. We shall use a novel modelling method based on our previous research.

An unparalleled technology to be developed in the project is the flexible and precise solid modelling of arbitrary topology and geometry, which is of primary importance in the implant design. And also, combining the characteristics of the new composite material with the computer model design is an advantage of the proposed software system.

Title: DNA Chip Design Program

Investigator: A/P Lin Feng

Funding: School of Computer Engineering, Emerging Technology Lab Fund, 2005

Description:

We propose a pioneering research program to build our own capability of designing DNA chips, through the development of a web-based server. DNA chip design is analogous to IC design: While the wafer manufacturers are fed with the large-scale integrated circuit designs and produce electronically functioning semiconductor chips, microarray, or DNA chip, makers rely on various genome-based and pharmacogenetic chip designs to fabricate, for example, biologically workable human genome microarrays. The DNA chip technology is empowering the scientific community to understand the fundamental aspects underlining the growth and development of life as well as to explore the genetic causes of anomalies occurring in the functioning of the human body. Capability of providing DNA chip makers and users with professional designs is of great market value.

Title: Extraction of protein and gene interactions from the MEDLINE database

Investigator: Asst Prof He Yulan

Funding: School of Computer Engineering

Description:

This project focuses on the extraction of protein and gene interactions from the MEDLINE database using statistical approaches. More specifically, it can be factored into three steps. First extract relevant textual fragments from literature abstracts using some shallow information-retrieval-based techniques; then generate structured representation, such as frame/slot architecture, of the contents of the fragments by performing semantic parsing or text understanding; finally, identify protein or gene interactions through automatically acquired extraction rules. In addition, such inter-actions between biological entities might be displayed in a network format such that users may follow the network links to retrieve relevant documents from which the relations were extracted and inferred in an interactive manner.

The work is of both theoretical and practical significance. First, the research will integrate NLP techniques and machine learning algorithms to offer a cost-effective approach to protein and gene interaction extraction. Second, the work will build an integrated tool that enables users to retrieve relevant documents in a more efficient and effective way.

Title: Smart Laboratory Initiative: The Virtual Lab Dashboard”, Embedded and Hybrid Systems Programme (Main Phase)

Investigator: A/P Ng See Kiong

Description:

Our Smart Bio-Laboratory project seeks to deploy smart technologies pervasively within the wet laboratory to facilitate bio-scientists in their daily experimental activities. In this project, we develop a “Virtual Lab Dashboard” (VLD) platform for ubiquitous local and remote monitoring and control in a smart bio-laboratory. We have implemented a prototype VLD system that employs wireless mobile computing, Java, and LAMP (Linux, Apache, MySQL, PHP/Perl/Python) technologies to enable lab users to access different bio-equipments at different locations in different modes, showing that current wireless and embedded technologies can be effectively utilized to create a unique smart work space for scientific experimentation and research in the wet laboratories.

Title: Structural biology of stem cell proteins

Investigator: A/P Prasanna R. Kolatkar

Collaborators: Ray Stevens /Peter Kuhn, Lab Scripps, La Jolla CA , USA

Description:

GIS has been involved with several interesting systems in various areas including stem cell biology. Much of the current work has focused on identifying potential players in various pathways involved in stem cell totipotency. Platforms such as microarrays and proteomics have been used to generate the initial data. The next logical step for a mechanistic understanding of these systems would be to determine and analyze high resolution three-dimensional structures of these proteins individually as well complexes involving other proteins or DNA. This information will allow a detailed understanding of the systems in hand and will lead to further investigations including possibly the design of inhibitors or drug compounds for those pathways which might have relevant disease association.

The objective of this project is to determine the structures of many transcription factors with significant relevance to human development. The structures of these proteins and protein-

protein as well as protein-DNA complexes will allow the detailed understanding of several interesting systems. X-ray crystallographic methods will be used to obtain high-resolution structures of these complexes that will show the molecular determinants of the binding events. This knowledge is highly useful for understanding the details of the binding as well as the ability to design inhibitors to block events implicated in disease pathways.

Title: Protein-Protein Interactions

Investigator: A/P Prasanna R. Kolatkar

Description:

My group is working with inferring protein interaction based on data from many sources such as domain fusion, text mining, databases with experimental information (DIP, BIND) and many others. There is a large amount of structural information that is also existent which hasn't been well integrated with the interaction databases created so far. We have just started to incorporate several features from databases such as PDB and SCOP into the PPDB. The first step is the validation of multiple domains existing on a single polypeptide chain using structural information. This was done as mentioned in the previous section. We used this information to look at which domains on multi-domain chains represent the best Rosetta stones and thus decrease the number of false positives. Next we will expand the use of this structural data to multiple chain interactions and also interacting proteins. The comparison between multiple chain domain-domain interactions with single chain domain-domain interactions will also give us a better understanding of similarities and differences. We will also compare information from prokaryotic and eukaryotic data to assess the applicability of the structural information. The use of structural information will thus represent the bulk of the protein-protein interactions effort for the next phase. We will also be adding scoring functions to better annotate interactions which are more likely. The scoring functions which we will test include the use of nodal connectivity, local topology and global topology. This type of scoring scheme has been applied to yeast 2 hybrid data but we will apply to our predicted interactions based on various criteria.

Title: Distribution of mitochondrial NADH fluorescence lifetimes

Investigators: Ksenia Blinova, Stefanie Carroll, Salil Bose, Aleksandr V. Smirnov, John J. Harvey, Jay R. Knutson, and Robert S. Balaban

Collaborators: National Institutes of Health: National Heart Lung Blood Institute, Bethesda, USA, Chief: Dr. Robert S. Balaban

Description:

The lifetimes of fluorescent components of matrix NADH in isolated porcine heart mitochondria were investigated using time-resolved fluorescence spectroscopy. Three distinct lifetimes of fluorescence were resolved: 0.4 (63%), 1.8 (30%), and 5.7 (7%) ns (% total NADH). The 0.4 ns lifetime and the emission wavelength of the short component were consistent with free NADH. In addition to their longer lifetimes, the remaining pools also had a blue-shifted emission spectrum consistent with immobilized NADH. On the basis of emission frequency and lifetime data, the immobilized pools contributed >80% of NADH fluorescence. The steady-state kinetics of NADH entering the immobilized pools was measured in intact mitochondria and in isolated mitochondrial membranes. The apparent binding constants (K_{DS}) for NADH in intact mitochondria, 2.8 mM (1.9 ns pool) and >3 mM (5.7 ns pool), were on the order of the estimated matrix [NADH] (~3.5 mM). The affinities and fluorescence lifetimes resulted in an essentially linear relationship between matrix [NADH] and NADH fluorescence intensity. Mitochondrial membranes had shorter emission

lifetimes in the immobilized pools [1 ns (34%) and 4.1 ns (8%)] with much higher apparent K_{DS} of 100 μ M and 20 μ M, respectively. The source of the stronger NADH binding affinity in membranes is unknown but could be related to high order structure or other cofactors that are diluted out in the membrane preparation. In both preparations, the rate of NADH oxidation was proportional to the amount of NADH in the long lifetime pools, suggesting that a significant fraction of the bound NADH might be associated with oxidative phosphorylation, potentially in complex 1.

Title: Investigating electrostatic effects on DNA compaction: Applications to gene delivery and transcription regulation

Investigator(s): Prof Lars Nordenskiöld

Collaborator(s): Prof James Tam and A/P Liu Ding Xiang, School of Biological Sciences, NTU; A/P Alexander Lyubartsev, Stockholm University

Funding: University Research Committee (URC) (Academic Research Fund, MoE, Singapore), 2002 (PI); A*STAR Biomedical Research Council (BMRC) Singapore, 2003 (PI)

Description:

The specific aims are:

- (i) To experimentally determine the ability of different polyvalent ligands to condense DNA and other biopolyelectrolytes and how this depends on structural features of ligand and biopolymer.
- (ii) To establish the physical basis in terms of molecular interactions, for this condensation.
- (iii) To use this knowledge in the practical design of new gene delivery agents. Specifically, a new class of polyamine mimetics that are ϵ,δ -peptides will be developed.

To identify the electrostatic role in polyanion-polycation interaction of DNA with histone protein tails and other chromatin regulating proteins involved in transcriptional regulation

Title: Discovery of TFBS

Investigator: Asst Prof Bertil Schmidt

Collaborator: Wayne Mitchell, Genome Institute of Singapore

Description:

The sequencing of complete genomes from multiple organisms has revealed that most differences in organism complexity are due to elements of gene regulation that reside in intergenic regions. Both within and between species, transcriptional regulator binding sites (**TFBS**) and the proteins that recognize them govern the activity of cellular pathways that mediate adaptive responses and survival. Experimental identification of these regulatory elements is by nature a slow process. The availability of complete genomic sequences, however, opens the door for computational methods to predict binding sites and expedite our understanding of gene regulation at a genomic level. Just as with traditional experimental approaches, the computational identification of the molecular factors that control a gene's expression level has been problematic. As a case in point, the identification of putative motifs, which is the subject of this project, is a challenging computational task. For it, powerful new binding site finding algorithms and their implementation on high performance computers are required.

Title: Determination of transmembrane interhelical interactions and oligomerization using molecular dynamics simulations

Investigator: Asst Prof Jaume Torres

Description:

Interhelical interactions are explored using global searching molecular dynamics simulations. The target native interhelical interaction, provided it is included in the total conformational space searched, is one of many alternative models obtained.

One way we use to analyze the results from these simulations involves the use of homologous sequences. When the sequences are likely to share the same structure (identity > 50%), the only model that persists in all simulations using homologues turns out to be the correct one. Other models also present are eventually destabilized by some conservative mutation in one of the homologous sequences.

Additionally, when for every homologue sequence simulations are performed assuming different oligomeric sizes, this novel approach also solves another problem, which is to determine the number of subunits in a homooligomer. This is so because only if the oligomeric size is correct, a common model will be found for all homologous sequences.

Research Projects: Post Graduate Students

Title: Intelligent Web Mining Student: Do Tien Dung Advisor: A/P Hui Siu Cheung Project Period: 5 Nov 2003 – 4 Nov 2005
Title: Intelligent Instant Messaging Monitoring and Analysis System Student: Dong Haichao Advisor: A/P Hui Siu Cheung and Dr Chang KuiYu Project Period: 16 Mar 2004 – 16 Mar 2006
Title: Neural Systems Modeling with Functional Brain Imaging Student: Zheng Xue Bin Advisor: A/P Jagath C. Rajapakse Project Period: 6 Sep 2002 – 5 Sep 2005
Title: Fusion of Structural and Functional MR Images Student: Zhou Juan, Helen Advisor: A/P Jagath C. Rajapakse Project Period: 12 Feb. 2004 - 12 Feb. 2007
Title: High Performance Computing for Computational Biology Student: Du Zhihua Advisor: A/P Lin Feng Project Period: 13 Oct 2002 – 13 Oct 2005
Title: <i>In Silico</i> Modeling of Hormone-Regulated Gene Expression Network Student: Maria Stepanova Advisor: A/P Lin Feng and Dr Valerie Lin Project Period: Aug 2004 – Aug 2007
Title: Machine learning for microarray cancer classification Student: Shen Li Advisor: A/P Tan Eng Chong Project Period: July 2002 – Oct 2005
Title: Gene Selection for DNA Microarray Data Student: Zhou Xin Advisor: Dr Mao Kezhi Project Period: July 2002 – Sep 2005
Title: Feature Selection for Classification and Clustering Microarray Data Student: Nguyen Van Hien Advisor: Dr Vivekanand Gopalakrishnan and Dr Manoranjan Dash Project Period: 12 Jul 2004 – 12 Jul 2007

V. STAFF PUBLICATIONS AND IMPACT FACTOR

Books

1. **Limsoon Wong**, editor, "The Practical Bioinformatician", *Imperial College Press*, London, December 2003.
2. **Limsoon Wong**, editor, "The Practical Bioinformatician", *World Scientific*, New Jersey, May 2004.
3. Louxin Zhang, **Limsoon Wong**, editors. "Selected Topics in Post-Genome Knowledge Discovery", *Singapore University Press*, Singapore, May 2004.
4. **J. C. Rajapakse** and L. Wang, (eds.) "Neural Information Processing: Research and Development", *Springer - Verlag*, March 2004, ISSN 1434-9922, pp. 478.
5. Feng Chu and **Lipo Wang**, "Bio-medical data mining using neural networks", in *Encyclopedia of Data Warehousing and Mining*, John Wang (Editor), Information Sciences Publishing, 2005.
6. Yi-Ping Phoebe Chen, **Limsoon Wong**, editors, "Proceedings of the 3rd Asia-Pacific Bioinformatics Conference", *Imperial College Press*, London, January 2005.
7. A. Omondi and **J. C. Rajapakse**, (eds.) *FPGA Implementations of Neural Networks*, Kluwer Academic Publishers, Boston, 2005 (in press)

Journals

1. Corona, T., Bao, Q., Christ, N., Schwartz, T., **Jinming Li** and Droge, P., "Activation of site-specific integration in human cells by a single chain integration host factor", *Nucleic Acid Research*, Vol 31, No 17 (2003).
2. Korolev, N.; Lyubartsev, A. P.; Laaksonen, A.; and **Nordenskiöld, L.** "A Molecular Dynamics Simulation Study of Oriented DNA with Polyamine and Sodium Counterions. Diffusion and Averaged Binding of Water and Cations", *Nucl. Acid Res.*, 31 (20) 5971-5981, 2003.
3. Korolev, N., Lyubartsev, A., and **Nordenskiöld, L.** "Application of the Poisson Boltzmann Polyelectrolyte Model for Analysis of Thermal Denaturation of DNA in the Presence of Na⁺ and Polyamine Cations", *Biophys. Chem.*, 104, 55-66, 2003.
4. R. G. N. Meegama and **J. C. Rajapakse**, "NURBS-based segmentation of the brain in medical images," *International Journal of Pattern Recognition and Artificial Intelligence*, vol. 17, no. 6, pp 995-1009, 2003.
5. R.G. N. Meegama and **J. C. Rajapakse**, "NURBS snakes," *Image and Vision Computing*, 21 (2003) pp. 551-562.
6. W. Lu and **J. C. Rajapakse**, "Eliminating indeterminacy in ICA", *Neurocomputing*, 50, (2003), pp. 271 – 290.
7. M. N. Nguyen and **J. C. Rajapakse**, "Two-stage support vector machines for protein secondary structure prediction", *Neural, Parallel, and Scientific Computing*, Vol. 11, Issue 1 & 2, 2003.
8. **J. C. Rajapakse** and M. N. Nguyen, "General framework for two-stage approaches to protein secondary structure prediction", *Asia Pacific Biotech News*, vol. 7, no.3, 2003, pp. 122 – 128.
9. **J. C. Rajapakse**, "Book review: adaptive blind signal and image processing," *IEEE Transactions on Neural Networks*, vol. 14, no. 6, Nov. 2003, pp. 1580-1580.

10. **Guang-Bin Huang**, "Learning Capability and Storage Capacity of Two-Hidden-Layer Feedforward Networks", *IEEE Transactions on Neural Networks*, vol. 14, no. 2, pp. 274--281, 2003.
11. Wu, Z. K., **Lin, F.** and Seah, H. S., "Topology Preserving Voxelisation of Rational Bezier and NURBS Curves", *Computers & Graphics*, Vol. 27, No. 1, 2003.
12. Wu, Z. K., **Lin, F.** and Seah, H. S., "Tunnel-free Voxelisation of Rational Bezier Surfaces", accepted for publication in *The Visual Computer* journal, 2003.
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 38. S. L. Ho and **J. C. Rajapakse**, “High sensitive technique for translation initiation site detection,” *IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology*, San Diego, 2004.
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97. Haiquan Li, Jinyan Li, **Limsoon Wong**, Mengling Feng, Yap-Peng Tan, "Relative Risk and Odds Ratio: A Data Mining Perspective", *Proceedings of 24th ACM SIGMOD-SIGACT-SIGART Symposium on Principles of Database Systems*, pages 368--377, Baltimore, Maryland, June 2005.
98. **J. C. Patra**, L. Wang, E. L. Ang and N. S. Chaudhari, "Neural network-based analysis of DNA microarray data", *IEEE Intl. Joint Conf. Neural Networks*, Montreal, 2005. (accepted)
99. **J. C. Patra**, Q. Zhen, E. L. Ang and A. Das, Neural networks for gene expression analysis and gene selection from DNA microarray data", Accepted for presentation, *IEEE Intl. Joint Conf. Neural Networks*, Montreal, 2005.
100. **See-Kiong Ng** "Smart Bio-Laboratories of the Future", in *Proceedings of the IEEE International Symposium on Circuits and Systems (ISCAS)*, Kobe, Japan, May 23-26, 2005, pages 4779-4782.
101. Z. Zhuo, S. Tang, **See-Kiong Ng**, "Toward Discovering Disease-Specific Gene Networks", in *Proceedings of the 3rd Asia-Pacific Bioinformatics Conference (APBC-2005)*, 17-21 January, Singapore, pages 161-170.
102. W.-K. For, **See-Kiong Ng**, X. Bao, and W.-S. Gan, "Relative Proximity Estimation in a Confined Small-Scale Environment", accepted for the 2005 *International Workshop on Wireless Ad-Hoc Networks*, London, UK, May 23-26, 2005.
103. W.-K. For, X. Bao, W.-S. Gan, **See-Kiong Ng**, "Reconfigurable Context-Sensitive Bio-Bridge Middleware for Smart Bio-Laboratories", in *Proceedings of the 19th International Conference on Advanced Information Networking and Applications (AINA2005)*, 28-30 March 2005, Vol 2, pages 561-566.
104. Shen L. and **Tan, E. C.**, 'Nonlinear kernel MSE methods for cancer classification', *International Conference on Natural Computation (ICNC'05) and International Conference on Fuzzy Systems and Knowledge Discovery (FSKD'05)*, Changsha, China, 27-29 August 2005.
105. Shen L. and **Tan, E. C.**, 'PLS and SVD based penalized logistic regression for cancer classification using microarray data', *The 3rd Asia-Pacific Bioinformatics Conference (APBC 2005)*, Singapore, 17-21 January, 2005
106. Du, Z. H., Stamatakis, A., **Lin, F.**, Roshan, U. W., and Nakhleh, L., "Parallel Divide-and-Conquer Phylogeny Reconstruction by Maximum Likelihood", *The 2005 International Conference on High Performance Computing and Communications (HPCC-05)*, Capri-Sorrento Peninsular, Italy, September 21-24, 2005.
107. D. Wang and **G.-B. Huang**, "Protein Sequence Classification Using Extreme Learning Machine", *Proceedings of International Joint Conference on Neural Networks (IJCNN2005)*, Montreal, Canada, 31 July - 4 August, 2005.
108. N.-Y. Liang, P. Saratchandran, **G.-B. Huang**, and N. Sundararajan, "Cognitive mental task classification using a novel on-line learning algorithm", *9th International conference on Cognitive and Neural Systems*, Boston, May 18 – 21, 2005.
109. X. Wei, Y. Li, and **G.-B. Huang**, "Fault Diagnosis Based on Extreme Learning Machine and Support Vector Machines," the *IASTED International Conference on Computational Intelligence (CI 2005)*, Calgary, Canada, July 4-6, 2005.
110. D. Wang and **G.-B. Huang**, "Protein Sequence Classification Using Extreme Learning Machine", *Proceedings of International Joint Conference on Neural Networks (IJCNN2005)*, Montreal, Canada, 31 July - 4 August, 2005.

111. F. Han, D.-S. Huang, Y.-M. Cheung, and **G.-B. Huang**, “A New Modified Hybrid Learning Algorithm for Feedforward Neural Networks,” *the International Symposium on Neural Networks (ISNN2005)*, Chongqing, China, May 30 - June 1, 2005.
112. Gavyn Pang, **Jagath Rajapakse**, “Comparative Genomic study of Parkinson’s disease candidate genes” for the *International Joint Conference on Neural Networks (IJCNN2005)*, Montreal, Canada
113. Gavyn Pang, **Jagath Rajapakse**, “Inferring Neutral Evolution from Parkinson’s Disease Genes” for the *IEEE symposium on computational intelligence in Bioinformatics and computation biology*.
114. C. Chen, **B. Schmidt**, “Parallel Construction of Large Suffix Trees on a PC Cluster”, *Euro-Par 2005*, Lisbon, Portugal, LNCS, Springer, 2005.
115. M. Rajapakse, L. Wyse, **B. Schmidt**, V. Brusica, “Deriving Matrix of Peptide-MHC Interactions in Diabetic Mouse by Genetic Algorithm”, *6th International Conference on Intelligent Data Engineering and Automated Learning (IDEAL 2005)*, Brisbane, Australia, LNCS, Springer, 2005.
116. T. Oliver, **B. Schmidt**, D. Nathan, R. Clemens, D. Maskell, “Multiple Sequence Alignment on an FPGA”, *11th International Conference on Parallel and Distributed Systems (ICPADS 2005) (Workshops)*, Fukuoka, Japan, 2005.
117. T. Oliver, **B. Schmidt**, D. Maskell, A.P. Vinod, “A Reconfigurable Architecture for Scanning Biosequence Databases”, *IEEE International Symposium on Circuits and Systems (ISCAS 2005)*, Kobe, Japan, 2005.
118. W. Liu, **B. Schmidt**, “A Case Study on Pattern-based Systems for High Performance Computational Biology”, *19th IEEE International Parallel & Distributed Processing Symposium (IPDPS 2005) (Workshops)*, Denver, CO.
119. T. Oliver, **B. Schmidt**, D. Maskell, “Hyper Customized Processors for Bio-Sequence Database Scanning on FPGAs”, *13th ACM International Symposium on Field-Programmable Gate Arrays, (FPGA 2005)*, Monterrey, CA, 2005.
120. T. Liu, **B. Schmidt**, “Optimal local alignment in RNA secondary structures”, *IASTED International Conference on Biomedical Engineering (BioMED 2005)*, Innsbruck, Austria, 2005.

VI. POSTGRADUATE STUDENTS COMPLETED

PhD Students

No	Name	Supervisor	Previous degree	Year Graduated	Placement
1	Dr Tan Choong Leong	A/P Jagath Rajapakse	PhD Eng, NTU	2003	Senior Engineer, Mtouche Pte Ltd, Singapore
2	Dr. R. G. N. Meegama	A/P Jagath Rajapakse	PhD Eng, NTU	2004	Senior Lecturer and Director, Centre for Computing Services, University of Sabaragamuwa, Sri Lanka.
3	Dr. W. Lu	A/P Jagath Rajapakse	PhD Eng, NTU	2003	Senior Engineer, Sony Research Labs, Singapore.
4	Palasingam Paaventhan	A/P Prasanna Kolatkar	PhD, NUS, Dept of Biological Science	2005	

MSc Students

No	Name	Supervisor	Previous degree	Year Graduated	Project Title
1	Yang Kanyan	A/P Jagath Rajapakse	MSc	2005	Brain connectivity with ICA
2	H. P. Ong	A/P Jagath Rajapakse	MEng.	2003	Image analysis using fuzzy networks
3	V. Venkatraman	A/P Jagath Rajapakse	MEng	2003	Neural network modeling of nonlinear response in fMRI
4	Jia Yiyu	A/P Kwoh Chee Keong	MSc	2004	Statistical analysis of intron phases at the splice sites of eukaryotic genes
5	Zhao Ying	A/P Kwoh Chee Keong	MSc	2004	Probabilistic based algorithm to analyze gene expression data
6	Feng Yuan	A/P Ng See Kiong	MSc, NUS	2005	Web services and NLP
7	For Wei Khing	A/P Ng See Kiong	MEng, NTU	2005	Enabling Location Awareness with Automatic-Reprogrammable Context-Sensitive Bio-Bridge Middleware for Smart Bio-Laboratories

VII. PRESTIGE

Professional Activities

No.	Title	Staff Name	Organization
1	Committee Member	A/P Jagath Rajapakse	IEEE Singapore Chapter, Engineering in Medicine and Biology Society, 2004 – present.
2	Steering Committee	A/P Jagath Rajapakse	European Conference on Evolutionary Computations and Machine Learning in Biology (EvoBIO), (April 2005 - present)
3	Technical Committee	A/P Jagath Rajapakse	Bioinformatics and Bioengineering (BBTC), IEEE Computational Intelligence Society, Nov. 2004 – present.
4	Vice Chair, Technical Committee	A/P Jagath Rajapakse	Pattern Recognition for Bioinformatics, International Association of Pattern Recognition (IAPR), Nov. 2004 – Nov. 2006.
5	Senior Member	A/P Jagath Rajapakse	Institute of Electrical and Electronic Engineers (IEEE)
6	Governing Board Member	A/P Jagath Rajapakse	Asia Pacific Neural Network Assembly (APNNA)
7	Technical Committee on Neural Networks	A/P Jagath Rajapakse	The International Association of Science and Technology for Development (IASTED) (2003 - 2006)
8	International Advisory Board	A/P Jagath Rajapakse	Knowledge Engineering and Discovery Research Institute, Auckland University of Technology
9	Steering Committee	A/P Jagath Rajapakse	Independent Component Analysis (ICA) Conferences
10	Committee Member	A/P Wong Lim Soon	Tan Kah Kee-DSTA Defense Science Award Committee (2003)
11	Management Committee	A/P Wong Lim Soon	National University of Singapore Institute of Engineering Science (2004-2005)
12	Board of Directors	A/P Wong Lim Soon	Association of Asian Societies for Bioinformatics (2003)
13	Board of directors	A/P Wong Lim Soon	Molecular Connections, Bangalore, India
14	SAB	A/P Wong Lim Soon	geneticXchange inc, California, USA
15	Chairman	A/P Wong Lim Soon	A*STAR Tech Scan Panel on Information Management
16	Member	Dr Salil K Bose	New York Academy of Sciences
17	Member	Prof Lars Nordenskiöld	NTU Working Group on Quality Assurance in Teaching, 2003
18	Coordinator	Prof Lars Nordenskiöld	25% joint appointment with Division of Bioengineering, coordinator for SBS teaching in the Bioengineering course, 2004

No.	Title	Staff Name	Organization
19	Senior Member	Asst/P Huang Guangbin	Institute of Electrical and Electronic Engineers (IEEE)
20	Member	Asst/P Liu Jianjun	Domain-Specific Review Board C, National Health Group, Singapore
21	Member	Asst/P Liu Jianjun	Peripheral, Central, Sensory & Cellular Nervous System/Mental Health Subcommittee, National Medical Research Council, Singapore

Conference Activities

No.	Title	Staff Name	Activity
1	Technical Program Committee	A/P Jagath Rajapakse	First IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, October, 2004
2	International Program Committee	A/P Jagath Rajapakse	4th Symposium of Independent Component Analysis and Blind Signal Separation (ICA2004), Granada, Spain, 2004.
3	International Program Committee	A/P Jagath Rajapakse	3 rd Symposium of Independent Component Analysis and Blind Signal Separation (ICA2003), Japan, 2003.
4	Program Committee	A/P Jagath Rajapakse	7 th IASTED International Conference on Computers, Graphics, and Imaging, CGIM 2004, August 2004, Hawaii, USA.
5	Program Committee	A/P Jagath Rajapakse	6 th IASTED International Conference on Computers, Graphics, and Imaging, CGIM 2003, August 2003, Hawaii.
6	Program Co-Chair	A/P Jagath Rajapakse	IEEE Symposium on Bioinformatics and Computational Biology (CBB) Honolulu, Hawaii, April, 2007.
7	Program Co-Chair	A/P Jagath Rajapakse	First International Workshop on Pattern Recognition in Bioinformatics (PRIB'06), Hong Kong, August 2006.
8	Publicity Chair	A/P Jagath Rajapakse	Fourth European Workshop on Evolutionary Computation in Bioinformatics (EvoBio'06), Budapest, Hungary, April 10 – 12, 2006.
9	International Program Committee	A/P Jagath Rajapakse	2005 International Conference on Machine Learning and Applications (ICML'05), Los Angeles, CA, December 15-17, 2005.
10	Publicity Co-Chair	A/P Jagath Rajapakse	IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, November, 2005

No.	Title	Staff Name	Activity
11	Technical Program Committee	A/P Jagath Rajapakse	IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, November, 2005
12	Advisory Committee	A/P Jagath Rajapakse	12 th International Conference on Neural Information Processing ICONIP2005, Taipei, Taiwan, November 2005.
13	Program Committee	A/P Jagath Rajapakse	BIOINFO2005 (International Joint Conference of AASBi, InCoB, and KSBI), Busan, Korea, September 2005.
14	International Program Committee	A/P Jagath Rajapakse	International Conference on Computer Graphics and Imaging (CGIM 2005), Honolulu, Hawaii, August 2005
15	International Program Committee	A/P Jagath Rajapakse	IASTED International Conference on Computational Intelligence, Calgary, Canada, July 2005
16	Program Committee	A/P Jagath Rajapakse	First International Conference on Complex Medical Engineering (CME 2005) , Takamatsu, Japan, May 15 -- May 18, 2005
17	Program Committee	A/P Jagath Rajapakse	3rd European Workshop on Evolutionary Bioinformatics, Lausanne, Switzerland, March 30 – April 1, 2005
18	Program Committee	A/P Jagath Rajapakse	Graduate Student Satellite Symposium: Asia Pacific Bioinformatics Conference (APBC05), Singapore, 15 January 2005
19	International Program Committee	A/P Jagath Rajapakse	2 nd IASTED conference on Neural Networks and Computational Intelligence, Grindelwald, Switzerland (NCI 2004), Feb 2004
20	Program Committee	Asst/P Vivekanand Gopalkrishnan	5th International Conference on Web-Age Information Management (WAIM'2004)
21	Scientific Committee	A/P Shu Jian Jun	The 1st International Conference “From Scientific Computing to Computational Engineering” Athens, Greece (8 – 10 September 2004)
22	Program Committee	A/P Ng See Kiong	16 th International Conference on Genome Informatics (GIW-2005), Yokohama, December 19-21, 2005.
23	Regional Chair	A/P Ng See Kiong	BIOINFO2005 (a joint event comprising INCOB2005, AASBi2005 and KSBi2005) in Busan, South Korea, September 22-24, 2005.
24	Program Committee	A/P Ng See Kiong	1 st International Symposium on Semantic Mining in Biomedicine, European Bioinformatics Institute (EBI) in Hinxton, Cambridge, UK, April 10-13, 2005.

No.	Title	Staff Name	Activity
25	Program Committee	A/P Ng See Kiong	1 st International Workshop on Data Mining and Bioinformatics (in conjunction with the 2005 International Conference on Computational Science and Its Applications), Singapore, May 9-12, 2005.
26	Program Committee	A/P Ng See Kiong	3 rd Asia Pacific Bioinformatics Conference (APBC-2005), Singapore, 17-21 January, 2005.
27	Program committee and Best Paper Judge	A/P Ng See Kiong	15 th International Conference on Genome Informatics (GIW-2004), Yokohama, Japan, December 13-15, 2004.
28	Program committee	A/P Ng See Kiong	BioLINK Workshop, HLT/NAACL 2004, Boston, USA, May 6, 2004.
29	Program committee	A/P Ng See Kiong	Text Mining in Biomedicine Thematic Session, 1 st International Joint Conference of Natural Language Processing (IJCNLP-2004), Hainan, China, March 22-24, 2004.
30	Track chair	Asst/P Huang Guangbin	The 5 th International Conference on Information, Communications and Signal Processing (ICICS 2005), Bangkok, Thailand, 6-9 December, 2005
31	Program Committee	Asst/P Huang Guangbin	International Symposium on Neural Networks, China 2006
32	Program Committee	Asst/P Huang Guangbin	The 2005 International Conference on Intelligent Computing (ICIC2005), Hefei, China, August 18-21, 2005.
33	Program committee	Asst/P Huang Guangbin	The International Conference on Electrical and Electronics Engineering (ICEEE) and XI Conference on Electrical Engineering (CIE 2005) (ICEEE-CIE 2005), Mexico City, Sept 7-9, 2005.
34	Program Committee	Asst/P Huang Guangbin	The 11 th International Conference on Neural Information Processing (ICONIP 2004), Calcutta, India, November 22-25, 2004

Editorial Services

No.	Title	Staff Name	Activity
1	Editorial Board Member	A/P Jagath Rajapakse	International Journal of Computational Intelligence
2	Editorial Board Member	A/P Jagath Rajapakse	Neural Information Processing - Letters and Reviews
3	Guest Co-Editor	A/P Jagath Rajapakse	Special Issue on “Computational Intelligence Approaches in Computational Biology and Bioinformatics”, IEEE Transactions on Computational Biology and Bioinformatics, (to appear in late 2006).
4	Guest Co-Editor	A/P Jagath Rajapakse	Special Issue on “Softcomputing in Bioinformatics and Medical Informatics”, Softcomputing, Springer (to appear in late 2005)
5	Guest Editor	Ast/P Sourav Bhowmick	Special Issue, Data and Knowledge Engineering Journal, Elsevier Science
6	Associate Editor	A/P Wang Lipo	IEEE Transactions on Neural Networks, 2002 -
7	Associate Editor	A/P Wang Lipo	IEEE Transactions on Evolutionary Computation, 2003
8	Editorial Board Member	A/P Wang Lipo	Soft Computing, 2002
9	Editorial Board Member	A/P Wang Lipo	Neural Information Processing – Letters and Reviews, 2003
10	Associate Editor	Prof Lars Nordenskiold	Biophysical reviews and Letters
11	Series Editor	A/P Wong Lim Soon	Advances in Bioinformatics & Computational Biology (book series) (2004)
12	Editor	A/P Wong Lim Soon	International Journal of Information Technology
13	Managing Editor	A/P Wong Lim Soon	Journal of Bioinformatics & Computational Biology
14	Advisor	Dr Salil K. Bose	Editorial Board of Journal of Biology Education, UK
15	Associate Editor	A/P Ng See Kiong	Advances in Bioinformatics and Computational Biology” (ABCB) book series, Imperial College Press, London, 2004.

Staff Awards

No.	Staff	Awards
1	A/P Wong Lim Soon	2003 FEER Asian Innovation Gold Award
2	A/P Jagath Rajapakse	Asian/American Who's Who, 2003 onwards
3	A/P Jagath Rajapakse	Who's Who in American Education, 2003 onwards

Student Awards

No.	Student / Supervisor	Awards
1	Ho Sy Loi / A/P Jagath Rajapakse	50,000 yen by Japanese Bioinformatics Society for the work presented at GIW2003 Splice site detection with a higher-order Markov model implemented on a neural network.
2	Minh Nguyen Ngoc / A/P Jagath Rajapakse	50,000 yen by Japanese Bioinformatics Society for the work presented at GIW2003: Multi-class Support Vector Machines for Protein Secondary Structure Prediction.
3	Yang Xiao and A/P Jagath C. Rajapakse	Nominee for the Best Paper Award, International Conference of Genomic Informatics (GIW2004), Yokohama, Dec. 2004
4	Ho Sy Loi / A/P Jagath Rajapakse	Best Overall Paper Award, IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, Oct 2004
5	Ho Sy Loi / A/P Jagath Rajapakse	Best Student Paper Award, IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, San Diego, Oct 2004
6	Wong Chia Sern / A/P Lin Feng	Industrial Attachment student working on Advanced Planning and Decision System and Multiple Path Finder, won the Silver Award at the DSTA Best Projects Competition, 2005.

VIII. PATENTS AND COMMERCIAL PRODUCTS

No.	Staff Name	Patents
1	Ast/P Fong Cheuk Ming	International patents filed by the Motorola IP Law Department in 1999-2000 for innovations incorporated into our Mobilepad™ range of handheld wireless communication products.
2	A/P Prasanna Kolatkar	The use of a fungal immunomodulatory protein, Fve, for immunotherapy, against allergy, virus infection and cancer.

No.	Staff Name	Commercial Products
1	Ast/P Sourav Bhowmick	Research in biological data integration has been adopted and implemented in the commercial product gRNA now marketed by Genvea BioSciences, Singapore (previously marketed by HeliXense Pte Ltd, Singapore)

IX. PERFORMANCE INDICATORS

Impact Factors

Impact factors for Years 2003-2005 (years with available data):

	2003	2004	2005
Total Impact	53.189	80.742	78.75
Number of Journal Papers	25	30	31
Number of Staff*	31	30	33
Number of Academic Staff	23	23	25
Impact factor per Journal Paper	2.13	2.69	2.54
Impact factor per Staff*	1.72	2.69	2.39
Impact factor per Academic Staff	2.31	3.51	3.15

*Staff includes both academic and research staff except research students.
Research staff includes RF, RA and PO, regardless of the funding source.

X. BIRC STAFF

Director:	A/P Liao Kin
Deputy Directors:	A/P Cai Yiyu A/P Jagath C. Rajapakse
MSc Programme Directors:	A/P Kwoh Chee Keong A/P Lin Feng
Executive Officer:	Ms. Norhana Ahmad
Research Fellows:	Dr Duan Kaibo Dr Ma Jianmin Dr Susanta Mukhopadhyay Dr Wang Yang
Project Officers:	Mr. Pang Wei Lai Mr. Ho Sy Loi Miss Keren-Happuch E Fan Fen Mr. Nguyen Ngoc Minh
Technical Executives:	Mr. Toh Wan Quan Ms. Wong Lee Chin

XI. COLLABORATORS

The centre brings together scientists and engineers, who are interested in bioinformatics modeling and computation, and fosters cross-disciplinary interactions among different schools at NTU to perform advanced research in bioinformatics. It also makes the necessary partnerships with other research and educational institutions, locally and abroad, to achieve its objectives.

International Collaborators

1. Brain Science Institute, RIKEN, Japan
2. Knowledge Engineering and Discovery Research Institute (KEDRI), Auckland University of Technology
3. Bioimaging Centre, Whitehead Institute, Massachusetts Institute of Technology (MIT), USA
4. Signal & Image Processing Group, Max-Planck-Institute of Cognitive Neuroscience, Germany
5. RMIT University, Melbourne, Australia
6. Stockholm University, Sweden
7. The Children's Hospital Research Foundation, Cincinnati Children's Hospital Medical Centre, USA
8. Department of Neurology, University of Freiburg, Germany
9. National Heart Lung Blood Institute, Bethesda, USA
10. Lab Scripps, La Jolla CA , USA
11. University of Leipzig, Germany
12. Institute of Cytology and Genetics, Russian Academy of Sciences, Novosibirsk, Russia
13. School of Molecular Biosciences, Washington State University, USA
14. University of Ulster Jordantown, North Ireland
15. Department of Bioscience and Bioinformatics, Kyushu Institute of Technology, Japan

Local Collaborators

1. Bioinformatics Institute (BII)
2. Genomic Institute of Singapore (GIS)
3. Institute of Infocomm Research (I2R)
4. National Neuroscience Institute (NNI)
5. Singapore General Hospital (SGH)
6. National Cancer Centre (NCC)
7. Tan Tock Seng Hospital (TTSH)
8. Mount Elizabeth Hospital
9. National University of Singapore (NUS)