

# The Fourth International Conference on Computational Systems Biology (ISB 2010)

## Local Organizer



## Organizers



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**September 9-11, 2010  
Suzhou, Jiangsu, China**

# ISB2010 Schedule

September 8 Wednesday	15:00-23:30	Registration (hotel lobby at Gusu Hotel)		
	18:00-19:30	Welcome reception (Gusu hotel)		
	19:30-21:30	Board members meeting of Society of Computational Systems Biology (Room #2 in Suzhou hotel)		
September 9 Thursday	08:30-08:40	Opening Session(Main Conf Room of Red building Conference center of Soochow University)		
	08:40-10:20	ISB Plenary Session P1(Main Conf Room of Red building Conference center of Soochow University)		
	10:20-10:50	Coffee break		
	10:50-12:30	ISB Plenary Session P2(Main Conf Room of Red building Conference center of Soochow University)		
	12:30-14:00	Lunch (Packed meal at conference site)		
	13:30-15:10	ISB Session A1 (Conf Room 201)	ISB Session B1 (Conf Room 217)	
		Dynamics of Bio-molecular Networks I	Bio-molecular Networks Analysis I	
	15:10-15:40	Coffee break		
	15:40-17:40	ISB Session A2 (Conf Room 201)	ISB Session B2 (Conf Room 217)	
		Computational Systems Biology I	Disease Systems Biology	
18:00-22:30	Dinner (Gusu hotel) & Night tour to Ancient Canal			
September 10 Friday	08:30-10:10	ISB Session A3 (Conf Room201)	ISB Session B3 (Conf Room 217)	
		Metabolic network and pathway	Bio-molecular Networks Analysis II	
	10:10-10:40	Coffee break		
	10:40-12:20	ISB Session A4 (Conf Room 201)	ISB Session B4 (Conf Room 217)	
		Computational Systems Biology II	Dynamics of Bio-molecular Networks II	
	12:30-14:00	Lunch (Packed meal at conference site)		
	13:30-14:20	ISB Plenary Session P3(Main Conf Room of Red building Conference center of Soochow University)		
	14:20-15:00	Coffee break		
	15:00-17:30	ISB Panel Discussion(Main Conf Room of Red building Conference center of Soochow University)		
Frontier in Computational Systems Biology				
18:00-20:00	Banquet & Performance			
September 11 Saturday	08:00-18:00	One day excursion in Suzhou		

# ISB 2010 Program

September 9-11, Suzhou, Jiangsu, China

## September 8 (Wednesday) Registration

**15:00-23:30 Registration**, Participants arrival in Suzhou, check in Gusu Hotel, and Registration package pick up (Hotel Lobby at Gusu Hotel).

**18:00-19:30 Welcome Reception** (Gusu hotel)

**19:30-21:30 Board member Meeting of Society of Computational Systems Biology of ORSC** (Meeting Room #2 in Suzhou hotel)

## September 9 (Thursday) Technical sessions

**08:00-11:30 Registration for late arrivals** (*Red building Conference center of Soochow University*)

**08:30-08:40 Opening Session** (Main Conf Room of Red building Conference center of Soochow University)

**8:40-10:20 ISB Plenary Session P1** (Main Conf Room of Red building Conference center of Soochow University)

**Chair: Luonan Chen**

**8:40-9:30** *Data Compression-Based Approaches to Analysis of Biological Networks*

**Tatsuya Akutsu**

Bioinformatics Center, Institute for Chemical Research, Kyoto University, Japan

**9:30-10:20** *Computing probability landscape of stochastic networks through Discrete Chemical Master Equation: Understanding Maintenance of Epigenetic State of Phage Lambda*

**Jie Liang**

Dept. of Bioengineering, University of Illinois at Chicago, USA

**10:20-10:50 Coffee break**

**10:50-12:30 ISB Plenary Session P2** (Conf Room #1)

**Chair: Xiang-Sun Zhang**

**10:50-11:40** *Integrative Analysis of Heterogeneous Genomics Data*

**Xianghong Jasmine Zhou**

University of Southern California, Los Angeles, USA

**11:40-12:30** *Random but Reliable: Properties of Spike Sequences of IP3-induced Ca<sup>2+</sup> signaling*

**Martin Faleke**

Mathematical Cell Physiology, Max Delbrück Centre for Molecular Medicine, Germany

**12:30-13:30 Lunch break**

**13:30-15:10 ISB Session A1** (Conf Room 201 of Red building Conference center of Soochow University)

**Topic: Dynamics of Biomolecular networks I**

**Chair: Martin Falcke**

**13:30-13:50** *A Mathematical Model of Fas Signaling Induced Apoptosis*

Chang Gu, Junjie Zhang, Yingyu Chen, **Jinzhi Lei**

Zhou Pei-Yuan Center for Applied Mathematics, Tsinghua University, Beijing 100084, China

**13:50-14:10** *Delay Discrete Dynamical Models for Genetic Regulatory Networks*

**Hao Jiang**, Wai-Ki Ching, Kiyoko F. Aoki-Kinoshita, DianJing Guo

Advanced Modeling and Applied Computing Laboratory, Department of Mathematics, The University of Hong Kong, Hong Kong, China

**14:10-14:30** *Modeling the Dynamics of the XlnR Regulon Network in Aspergillus nige*

**Jimmy Omony**, Leo H. de Graaff, Gerrit van Straten, Anton J.B. van Boxtel

Systems and Control group, Wageningen University, P.O. Box 17, 6700 AA Wageningen, The Netherlands

**14:30-14:50** *Property of Multiple Equilibria for SSI Metabolic Module*

**Hong-Bo Lei**, Ji-Feng Zhang

Key Laboratory of Systems and Control, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, P. R. China

**14:50-15:10** *Adaptive Unscented Kalman Filter for Estimation of Parameters in Kinetic Metabolic Models*

**Syed Murtuza Baker**, Bjorn H. Junker

Leibniz Institute of Plant Genetics and Crop Plant Research, 06466 Gatersleben, Germany

**13:30-15:10 ISB Session B1** (Conf Room 217 of Red building Conference center of Soochow University)

**Topic: Biomolecular Networks Analysis I**

**Chair: Xianghong Jasmine Zhou**

**13:30-13:50** *Cross-species Functional Conservation and in silico Gene Replacement for HIF Pathways*

Chia-Sheng Chuang, Chih-Chia Chen, **Tun-Wen Pai**, Chin-Hua Hu, **Hao-Teng Chang**, Margaret Dah-Tsyng Chang

Department of Computer Science and Engineering, National Taiwan Ocean University, Keelung, Taiwan

**13:50-14:10** *Significant Regulatory Networks from Goto-Kakizaki Rat Liver Microarray Data during Diabetic Progression*

**Huarong Zhou**, Shigeru Saito, Guanying Piao, Rongkuan Hu, Jiguang Wang, Zhi-Ping Liu, Katsuhisa Horimoto

Key Laboratory of Systems Biology, SIBS-Novo Nordisk Translational Research, Centre for PreDiabetes, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai 200233, China

**14:10-14:30** *On Construction of Sparse Probabilistic Boolean Networks from a Prescribed Transition Probability Matrix*

**Lu-Bin Cui**, Wen Li, Wai-Ki Ching

School of Mathematical Sciences, South China Normal University, Guangzhou 510631, China

**14:30-14:50** *Uncover the Transient Transcriptional Regulations by a Novel Sliding Window*

*Correlation Strategy*

**Jiguang Wang**, Yong Wang, Xianwen Ren, Wei Guo, Luonan Chen  
Academy of Mathematics and Systems Science, Chinese Academy of Science, Beijing, China

**14:50-15:10** *Conditional Random Field Approach to Prediction of Protein-Protein Interactions Using Mutual Information Between Domains*

**Morihiro Hayashida**, Mayumi Kamada, Jiangning Song, Tatsuya Akutsu  
Bioinformatics Center, Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto, 611-0011, Japan

**15:10-15:40 Coffee break**

**15:40-17:40 ISB Session A2** (Conf Room 201 of Red building Conference center of Soochow University)

**Topic: Computational Systems Biology I**

**Chair: Tatsuya Akutsu**

**15:40-16:00** *Computational Analysis of Protein Tyrosine Nitration*

ZhiSong He, **Tao Huang**, XiaoHe Shi, LeLe Hu, Lei Chen, Fang Liu, Kai Wang, TieQiao Wen, XiangYin Kong, Yudong Cai  
Key Laboratory of Systems Biology, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai 200031, China

**16:00-16:20** *Identifying Protein Binding Hot Spots by Using Deeply Buried Atomic Contacts*

**Zhenhua Li**, Jinyan Li  
Bioinformatics Research Center, School of Computer Engineering, Nanyang Technological University, Nanyang Avenue, Singapore 639798

**16:20-16:40** *A Measure for Sequence Similarity Based on Dual Nucleotides and Information Discrepancy*

Zhen Wang, **Jia-Wei Luo**, Han-Qi Zhou, Fang Liu  
School of Computer and Communication, Hunan University, Changsha, Hunan Province, 410082

**16:40-17:00** *Genome-wide Analysis of the Transcription Factor Binding Preference of Human Bidirectional Promoters and Functional Annotation of the Related Gene Pairs*

Bingchuan Liu, Jiajia Chen, **Bairong Shen**  
Center for Systems Biology, Soochow University, Suzhou, 215006, China

**17:00-17:20** *MetaDBSite: a Meta Approach to Improve Protein DNA-Binding Sites Prediction*

**JingNa Si**, **Zengming Zhang**, Biaoyang Lin, Michael Schroeder, **Bingding Huang**  
Systems Biology Division, Zhejiang-California International NanoSystems Institute, Zhejiang University, Kaixuan Road 268, 310029, Hangzhou, China

**17:20-17:40** *Effects of Multiple Probesets in Affymetrix GeneChips on Identifying Differentially Expressed Genes in iPS Cells*

**Zhi-Ping Liu**, Xiang-Sun Zhang  
Key Laboratory of Systems Biology, SIBS-Novo Nordisk Translational Research Center for Pre-diabetes, Shanghai Institutes for Biological Sciences, CAS, Shanghai 200031

**15:40-17:40 ISB Session B2** (Conf Room 217 of Red building Conference center of Soochow University)

**Topic: Disease Systems Biology**

**Chair: Tun-Wen Pai**

**15:40-16:00** *Predicting Cell Cycle Genes from E-MAP Profiles by Integrating Multiple Types of Data*

Wang Lin, Hou Lin, Minping Qian, Fangting Li, **Minghua Deng**

Center for Theoretical Biology, Peking University, Beijing

**16:00-16:20** *NRWRH for Drug Target Prediction*

**Xing Chen**, Gui-Ying Yan

Academy of Mathematics and Systems Science, Chinese Academy of Science, Beijing, China

**16:20-16:40** *Drug Target Identification Based on Flux Balance Analysis of Metabolic Networks*

Zhenping Li, Rui-Sheng Wang, **Xiang-Sun Zhang**

Academy of Mathematics and Systems Science, Chinese Academy of Science, Beijing, China

**16:40-17:00** *A Network Biology Approach to Understand Combination of Drugs*

**Ke-Jia Xu**, Jiangning Song, Xing-Ming Zhao

Institute of Systems Biology, Shanghai University, Shanghai 200444, China

**17:00-17:20** *A Network Target-based Approach for Evaluating Multicomponent Synergy*

Shao Li, Ningbo Zhang, **Bo Zhang**

MOE Key Laboratory of Bioinformatics and Bioinformatics Division, TNLIST /Department of Automation, Tsinghua University, Beijing 100084, China

**17:20-17:40** *Modelling of inquiry diagnosis for coronary heart disease in traditional Chinese medicine by using multi-label learning*

Guo-Ping Liu, **Guo-Zheng Li**, Ya-Lei Wang, Yi-Qin Wang

Department of Control Science & Engineering, Tongji University, Shanghai, 201804 China

**18:00-19:30 -Dinner at Gusu Hotel**

**19:30-22:30 The night tour to Ancient Canal of Suzhou**

## **September 10 (Friday) Technical sessions**

**8:30-10:10 ISB Session A3** (Conf Room 201 of Red building Conference center of Soochow University)

**Topic: Metabolic network and pathway**

**Chair: Xiufen Zou**

**08:30-08:50** *Addition of Autotrophic Carbon Fixation Pathways to Increase the Theoretical Heterotrophic Yield of Acetate*

Shuo-Huan Hsu, Priyan R. Patkar, Venkat Venkatasubramanian, **John A. Morgan**

School of Chemical Engineering, Purdue University, West Lafayette, IN 47907

- 08:50-09:10** *Network Flow Model Based Analysis of Mouse Hepatocarcinogenesis*  
Yu-Qing Qiu, Xing-Ming Zhao, Zikai Wu, Chaochao Wu, Rong Zeng, **Luonan Chen**  
Key Laboratory of Systems Biology, SIBS-Novo Nordisk Translational Research Center for Pre-diabetes, Shanghai Institutes for Biological Sciences, CAS, Shanghai 200031
- 09:10-09:30** *Impacts of Different Metabolite Measurement Protocols on Estimating Parameters in Complex Photosynthetic Carbon Metabolism Models*  
Wei Pan, John Fettig, Eric de Sturler, Xin-Guang Zhu  
Plant Systems Biology Group, Partner Institute of Computational Biology, Chinese Academy of Sciences/Max Planck Society, Shanghai 200031, China
- 09:30-09:50** *Three Faces of Metabolites: Pathways, Localizations and Network Positions*  
**Jing Zhao**, Petter Holme  
Department of Mathematics, Logistical Engineering University, Chongqing 400016, China
- 09:50-10:20** *An improved Kinetic Model for Acetone-Butanol-Ethanol Pathway of Clostridium acetobutylicum and Model-Based Perturbation Analysis*  
Ru-Dong Li, Yuan-Yuan Li, Ling-Yi Lu, Cong Ren, Yi-Xue Li, Lei Liu  
Key Laboratory of Systems Biology, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, China

**08:30-10:10 ISB Session B3** (Conf Room 217 of Red building Conference center of Soochow University)

**Topic: Bio-molecular Networks Analysis II**

**Chair: Katsuhisa Horimoto**

- 08:30-08:50** *Identification of Disease Locus Using Constrained Scaling Models*  
Yiu-Fai Lee, **Michael K. Ng**  
Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong
- 08:50-09:10** *Transcriptional Regulatory Network Discovery via Information Mining Approach in Rett Syndromes Study*  
**Xiaorong Yang**, Xianwen Ren, Xiaobo Zhou  
Center for Biotechnology & Informatics, The Methodist Hospital Research Institute, Weill Medical College, Cornell University, Houston, TX 77030, USA.
- 09:10-09:30** *Self-induced Stochastic Resonance in MicroRNA Regulation of a Cancer Network*  
Jianwei Shen, **Luonan Chen**, Kazuyuki Aihara  
Key Laboratory of Systems Biology, SIBS-Novo Nordisk Translational Research Center for Pre-diabetes, Shanghai Institutes for Biological Sciences, CAS, Shanghai 200031
- 09:30-09:50** *A Modified Entropy Approach for Construction of Probabilistic Boolean Networks*  
Xi Chen, Limin Li, Wai-Ki Ching, Nam-Kiu Tsing  
Advanced Modeling and Applied Computing Laboratory, Department of Mathematics, The University of Hong Kong, Hong Kong
- 09:50-10:20** *The Topological Properties of Virus-Human Protein Interaction Networks*  
Jinying Tan, Xiufen Zou  
School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China

**10:10-10:40 Coffee break**

**10:40-12:20 ISB Session A4** (Conf Room 201 of Red building Conference center of

Soochow University)

**Topic: Computational Systems Biology II**

**Chair: Ling-Yun Wu**

**10:40-11:00** *Constrained Subspace Clustering for Time Series Gene Expression Data*

**Jibin Qu**, Michael Ng, Luonan Chen

Academy of Mathematics and Systems Science, CAS, China

**11:00-11:20** *Functioning of the Brain*

Martin Vlcek

Ministry of Finance of the Czech Republic, Prague

**11:20-11:40** *GeneGo MetaCore/MetaDrug: Unique Systems biology platform for knowledge management and OMICs data analysis*

**Xiao Liu**

Tri-I Biotech(Shanghai) Inc.

**11:40-12:00** *Novel Global Network Scores to Analyze Kinase Inhibitor Profiles*

**Jacques Colinge**, Uwe Rix, Giulio Superti-Furga

CeMM – Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria

**10:40-12:20 ISB Session B4** (Conf Room 217 of Red building Conference center of Soochow University)

**Topic: Dynamics of Bio-molecular Networks II**

**Chair: Jie Liang**

**10:40-11:00** *Potential Linkages Between the Inner and Outer Cellular States of Human Induced Pluripotent Stem Cells*

Shigeru Saito, Yasuko Onuma, Yuzuru Ito, Hiroaki Tateno, Masashi Toyoda, Hidenori Akutsu, Koichiro Nishino, Emi Chikazawa, Yoshihiro Fukawatase, Yoshitaka Miyagawa, Hajime Okita, Nobutaka Kiyokawa, Yohichi Shimma, Akihiro Umezawa, Jun Hirabayashi, **Katsuhisa**

**Horimoto**, Makoto Asashima

Computational Biology Research Center, National Institute of Advanced Industrial Science Technology (AIST), 2-4-7 Aomi, Koto-ku, Tokyo 135-0064, Japan

**11:00-11:20** *Cell Signaling Dynamics Analysis in Leukemia with Switching Boolean Networks*

**Woochang Hwang**, Doheon Lee

Department of Bio and Brain Engineering, KAIST, Republic of Korea

**11:20-11:40** *Control of Directed Differentiation by Parameter Perturbations*

Xiao Chang, Deng Yu Liu, Zengrong Liu, Luonan Chen, Ruiqi Wang

Institute of Systems Biology, Shanghai University, Shanghai 200444, China

**11:40-12:00** *Nonlinear Dynamic Analysis of an Entermorpha prolifera Population Model*

Ying Li

College of Information Technology, Shanghai Ocean University, Shanghai 201306, China

**12:30-13:30 Lunch break**



**13:30-14:20 ISB Plenary Session P3** (Main Conf Room of Red building Conference center of Soochow University)

**Chair: Bairong Shen**

**13:30-14:20** *TBD*

**Hoong-Chien Lee**

University Chair Professor of Biophysics, Graduate Institute of Systems Biology and Bioinformatics, Department of Physics/ Graduate Institute of Biophysics, Center for Complex Systems, National Central University, Taiwan

**14:20-15:00 Coffee break**

**15:00-17:30 ISB Panel Discussion** (Main Conf Room of Red building Conference center of Soochow University)

**Topic: Frontier in Computational Systems Biology**

**Chair: Luonan Chen**

**18:00-20:00 Banquet & Performance**

**September 11 (Saturday)** Social Program: One-day tour to Suzhou city

**8:00** Departure at Gusu Hotel Lobby

\*The above program subjects to revision based on further information and Ad Hoc presentation requests.

# GeneGo MetaCore/MetaDrug: Unique Systems biology platform for knowledge management and OMICs data analysis

Xiao Liu

Tri-I Biotech(Shanghai) Inc. 源资信息科技（上海）有限公司

## Abstract:

At GeneGo, we believe that pathway analysis of inherently complex high-throughput biological and chemistry data must be based on a fundamental understanding of human and mammalian biology. That requires technology and expertise. Over the last 9 years, we have developed a unique approach of systems reconstruction™ for extracting invaluable knowledge from experimental articles and patents, structuring it in computer-readable form and storing in a semantically consistent database. The “knowledge”-derived data, represented as ontologies, protein interactions and gene-disease associations, signaling and metabolic pathways, normal and pathology process models, can then be used for functional analysis of OMICs datasets by a series of cheminformatics and bioinformatics software tools such as network generation algorithms, ontology enrichment, interactome calculations, pathway modeling, QSAR models etc.

To accommodate the complex aspects of mammalian functionality - such as coordinated expression of multiple genes to bring about a prescribed function, gene alleles in form of SNPs and mutations, RNA splice variants, protein isoforms, complexes, and families - GeneGo has developed a database of novel architecture. The key aspect of its data schema is semantic consistency between the entities from as different fields of study as human genetics, medicinal chemistry, toxicity, systems biology and translational medicine. This consistency, based on combining standard and proprietary ontologies, unique controlled vocabulary and a comprehensive ID system, enables application of sophisticated analytical and search tools such as MetaCore for pathway analysis and data mining, not available in public domain or from other vendors.

# Modelling of inquiry diagnosis for coronary heart disease in traditional Chinese medicine by using multi-label learning

Guo-Ping Liu, **Guo-Zheng Li**, Ya-Lei Wang, Yi-Qin Wang

## Abstract

**Background:** Coronary heart disease (CHD) is a common cardiovascular disease that is extremely harmful to humans. In Traditional Chinese Medicine (TCM), the diagnosis and treatment of CHD have a long history and ample experience. However, the non-standard inquiry information influences the diagnosis and treatment in TCM to a certain extent. In this paper, we study the standardization of inquiry information in the diagnosis of CHD and design a diagnostic model to provide methodological reference for the construction of quantization diagnosis for syndromes of CHD. In the diagnosis of CHD in TCM, there could be several patterns of syndromes for one patient, while the conventional single label data mining techniques could only build one model at a time. Here a novel multi-label learning (MLL) technique is explored to solve this problem.

**Methods:** Standardization scale on inquiry diagnosis for CHD in TCM is designed, and the inquiry diagnostic model is constructed based on collected data by the MLL techniques. In this study, one popular MLL algorithm, ML-kNN, is compared with other two MLL algorithms RankSVM and BPMLL as well as one commonly used single learning algorithm, k-nearest neighbour (kNN) algorithm. Furthermore the influence of symptom selection to the diagnostic model is investigated. After the symptoms are removed by their frequency from low to high; the diagnostic models are constructed on the remained symptom subsets.

**Results:** A total of 555 cases are collected for the modelling of inquiry diagnosis of CHD. The patients are diagnosed clinically by fusing inspection, pulse feeling, palpation and the standardized inquiry information. Models of six syndromes are constructed by ML-kNN, RankSVM, BPMLL and kNN, whose mean results of accuracy of diagnosis reach 77%, 71%, 75% and 74% respectively. After removing symptoms of low frequencies, the mean accuracy results of modelling by ML-kNN, RankSVM, BPMLL and kNN reach 78%, 73%, 75% and 76% when 52 symptoms are remained.

**Conclusions:** The novel MLL techniques facilitate building standardized inquiry models in CHD diagnosis and show a practical approach to solve the problem of labelling multi-syndromes simultaneously.