

## Message from the General Chair



Welcome to the First IEEE International Conference on Computational Advances in Bio and medical Sciences (ICCABS 2011)! Computational techniques are revolutionizing the way in which research is conducted in science and engineering. Unsurpassed advances have been made in myriads of application domains. This is particularly true in the areas of biology, medicine, and drug discovery. Even though a number of conferences exist today in the general area of bioinformatics, they focus on computational biology to a large extent. ICCABS has the goal of bringing together scientists in all the three areas and hence serving as a platform for bridging the research efforts in these areas. The response from these communities to the ICCABS call for papers has been indeed gratifying. I am honored to serve these international communities by bringing together researchers, scientists, and students from academia, laboratories, and industry to this premier meeting held in the ever exciting city of Orlando, FL.

I am extremely grateful to NSF for providing funds to support student travel awards, key note talks, etc. This support has helped the conference tremendously. I am thankful to the steering committee members (Srinivas Aluru, Reda A. Ammar, Tao Jiang, Vipin Kumar, Ming Li, John Reif, and Sartaj Sahni), Chun-Hsi Huang, Sushil K. Prasad, and Carmen P. Saliba who have been instrumental in getting this conference approved by IEEE.

I would like to thank Program Chairs Ion Mandoiu, Teresa Przytycka, and Satoru Miyano for assembling an outstanding technical program. The program committee members have done a wonderful job of reviewing all the submitted papers thoroughly within a short period of time. I am thankful to them as well as all the authors who have expressed their faith in ICCABS by submitting the fruits of their hard work. ICCABS features three keynote speeches (from Andrea Califano, Christina Leslie, and John Reif), and nine invited talks (from Paola Bonizzoni, Dan Brown, Oliver Eulenstein, Shinichi Morishita, Giri Narasimhan, Mihai Pop, Daniel Schwartz, Li-San Wang, and Alex Zelikovsky). I am grateful to these well-established and highly successful researchers for taking time out of their busy schedules to make ICCABS a great success.

Thanks are also due to: Financial Chairs (Reda Ammar and Chun-Hsi Huang), Local Arrangements Chair (Sumit Kumar Jha), Publicity Chair (Giri Narasimhan), Poster Chairs (Rachel O'Neill and Raj Sunderraman), Workshop Chairs (Dumitru Brinza, Raja Jothi, and Sing-Hoi Sze), and Proceedings Chairs (Jerlin Camilus Merlin and Sahar Al Seesi) for their tireless efforts. Ion Mandoiu and Alex Zelikovsky deserve my special thanks for putting together a great Workshop on Computational Advances for Next Generation Sequencing (CANGS 2011).

Selected papers from ICCABS 2011 will appear as special issues in BMC Genomics and BMC Bioinformatics. I am grateful to the editors of these journals and Vanessa MacDonald for their efforts in this regard. Last but not least, I would like to thank UConn and the Booth Engineering Center for Advanced Technology (BECAT) for the constant administrative support rendered to ICCABS. In particular, I offer my special thanks to Sandi Lizée for her incessant support.

I hope you'll continue to support ICCABS in future! Have a wonderful time in the conference!

*Sanguthevar Rajasekaran, University of Connecticut*

## Message from the Program Chairs



On behalf of the Program Committee, we would like to welcome you to the 1<sup>st</sup> IEEE International Conference on Computational Advances in Bio and medical Sciences (ICCABS 2011), held in Orlando, Florida on February 3-5, 2011. This year the technical program includes 36 extended abstracts selected by the Program Committee from a number of 89 full submissions received in response to the call for papers. The program also includes 9 invited talks and 34 poster presentations, and features keynote talks by three distinguished speakers. John Reif from Duke University speaks on DNA-based molecular devices, Andrea Califano from Columbia University speaks on a systems biology approach to integrative cancer genomics, and Christina Leslie from Memorial Sloan-Kettering Cancer Center speaks on high-resolution sequence and chromatin signatures in the human genome. Additionally, the technical program includes 13 invited talks presented as part of the 1<sup>st</sup> Workshop on Computational Advances for Next Generation Sequencing which is held in conjunction with ICCABS 2011.

We would like to thank the Program Committee members and external reviewers for volunteering their time to review and discuss submitted abstracts. We would like to extend special thanks to the General Chair, Sanguthevar Rajasekaran, for his leadership, and to the Local Organization, Proceedings, Finance, Publicity, and Posters Chairs for their hard work in making ICCABS 2011 a successful event. Last but not least we would like to thank all authors for presenting their work at the conference.

We hope you will find the ICCABS 2011 technical program interesting and thought provoking and that attending the conference will provide you with stimulating ideas and ample opportunities to meet other researchers from around the world. Enjoy!

*Ion Mandoiu*, University of Connecticut  
*Teresa Przytycka*, National Institutes of Health  
*Satoru Miyano*, University of Tokyo

## Message from CANGS Workshop Chairs



Welcome to the 1<sup>st</sup> Workshop on Computational Advances for Next Generation Sequencing (CANGS 2011), held on Friday, February 4, 2011 in Orlando, Florida in conjunction with ICCABS 2011. Massively parallel DNA and RNA sequencing have become widely available, reducing the cost by several orders of magnitude and placing the capacity to generate gigabases to terabases of sequence data into the hands of individual investigators. These next-generation technologies have the potential to dramatically accelerate biological and biomedical research by enabling the comprehensive analysis of genomes and transcriptomes to become inexpensive, routine and widespread.

The CANGS workshop aims to accelerate progress in the field by bringing together experts to discuss new directions of research and exchange ideas on the many mathematical and computational challenges presented by analysis of the exploding volume of next-generation sequencing data. This year's workshop program will span 3 sessions comprising 13 invited talks on a variety of current research topics, including error correction, genome and transcriptome assembly, molecular haplotyping, characterization of epigenetic factors and structural variants using next generation sequencing data, virus quasispecies reconstruction, and estimation of power in whole-genome sequencing studies. The workshop will conclude with a roundtable discussion of future research directions in the field.

We would like to thank ICCABS General Chair Sanguthevar Rajasekaran and ICCABS Workshop Chairs, Dumitru Brinza, Raja Jothi, and Sing-Hoi Sze, for the opportunity to organize CANGS 2011, and all speakers for presenting their work at the workshop.

*Ion Mandoiu*, University of Connecticut  
*Alex Zelikovsky*, Georgia State University

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# ICCABS 2011 Program

## Thursday, February 3, 2011

8:30am-  
8:40am **Opening Remarks**

8:40am-  
9:40am **Plenary Session**  
**Chair: Sanguthevar Rajasekaran**

Keynote talk: DNA-Based Molecular Devices  
*John Reif* (Duke University)

9:40am-  
10:00am **Coffee Break**

10:00am-  
12:00pm **Parallel Sessions**

**Session 1A: Invited talks**  
**Chair: Srinivas Aluru**

Invited talk: Fast and Theoretically Strong Algorithms for Kinship Discovery  
*Dan Brown* (University of Waterloo)

Invited talk: "Going Viral" with Biological Sequence Analysis  
*Daniel Schwartz* (University of Connecticut)

Invited talk: Comparative Microbial Genomics  
*Giri Narasimhan* (Florida International University)

**Session 1B: RNA and Protein Structure**  
**Chair: Sahar Elsis**

*Feng Lou And Peter Clote*. Maximum Expected Accurate Structural Neighbors of an RNA Secondary Structure  
*Yingfeng Wang, Amir Manzour, Pooya Shareghi, Timothy Shaw, Ying-Wai Li, Russell Malmberg and Liming Cai*. Stable Stem Enabled Shannon Entropies Distinguish Non-coding RNAs From Random Backgrounds  
*Nobuyoshi Mizoguchi, Yuki Kato and Hiroyuki Seki*. A Grammar-Based Approach to RNA Pseudoknotted Structure Prediction for Aligned Sequences  
*Naomi Fox and Ileana Streinu*. Redundant Interactions in Protein Rigid Cluster Analysis  
*Van Du Tran, Philippe Chassignet, Saad Sheikh and Jean-Marc Steyaert*. Energy-based Classification and Structure Prediction of Transmembrane Beta-Barrel Proteins  
*Tien-Hao Chang, Chih-Yun Chiang, Fung-Wei Lin and Chen-Yu Fan*. Studying Disorder-to-Order Transitions from Structural Analysis

12:00pm-  
1:20pm **Lunch**

1:20pm-  
3:20pm

## Parallel Sessions

### Session 2A: Invited talks

Chair: *Dan Brown*

Invited talk: Searching Massive Epigenome Data for Evolutionarily Conserved Sequence Motifs  
*Shinichi Morishita* (University of Tokyo)

Invited talk: Multiclass RNA Function Classification using Next-Generation Sequencing  
*Li-San Wang* (University of Pennsylvania)

Invited talk: Metabolic Network Alignments  
*Alex Zelikovsky* (Georgia State University)

### Session 2B: Genomics and Genetics

Chair: *Oliver Eulenstein*

*Aditya Varma, Abhiram Ranade and Srinivas Aluru*. An Improved Maximum Likelihood Formulation for Accurate Genome Assembly  
*Xing Yang, Daniel Medvin, Deborah Yoder-Himes, Stephen Lory and Giri Narasimhan*. CloG: a Pipeline for Closing Gaps in a Draft Assembly Using Short Reads  
*Jorge Duitama, Pramod Srivastava and Ion Mandoiu*. Towards Accurate Detection and Genotyping of Expressed Variants From Whole Transcriptome Sequencing Data  
*Yoon Soo Pyon, Matthew Hayes and Jing Li*. Model Based Clustering Approach for Identifying Structural Variation Using Next Generation Sequencing Data  
*Shawn O'Neil and Scott Emrich*. Robust haplotype reconstruction of eukaryotic sequence data with Hapler  
*Jiayin Wang, Jin Zhang and Yufeng Wu*. Identifying Interacting SNPs with Parallel Fish-Agent based Logic Regression

3:20pm-  
3:40pm

## Coffee Break

3:40pm-  
5:30pm

## Parallel Sessions

### Session 3A: Poster Overviews

Chair: *Rachel O'Neill*

- P1. *Cindy Grimm, Ruosi Li, Paul Heider, Alain Pierre Pierre and Rolf Mueller*. A Comparison of Local Shape Descriptors for Biological Applications  
P2. *Xiaoyong Sun, Ajith Gunaratne and Zhijun Wu*. PRDDs: A Protein Residue Distance&Angle Distribution Database for Secondary Structures  
P3. *Irina Astrovskaia, Bassam Tork, Serghei Mangul, Kelly Westbrooks, Ion Mandoiu, Peter Balfe and Alex Zelikovsky*. VISPA: Viral Spectrum Assembling Method  
P4. *Maryam Bijanzadeh, Rozita Jailani, M.Osman Tokhi and Samad.C Gharooni*. Development of Dynamic Leg Joint Model for Paraplegic with Functional Electrical Stimulation  
P5. *Jason Gallia, Anna Tan-Wilson and Patrick Madden*. De Novo Protein Identification by Dynamic

### Session 3B: Poster Overviews

Chair: *Daniel Schwartz*

- P18. *Juliana Tarossi Pollettini and Alessandra Alaniz Macedo*. Chronic Disease Prevention: A Translational Bioinformatics Approach  
P19. *Hsin-Wei Wang, Ya-Chi Lin, Hao-Teng Chang and Tun-Wen Pai*. Linear B-cell Epitope Prediction Based on Support Vector Machine and Propensity Scales  
P20. *Cing-Han Yang, Hsin-Wei Wang, Tsan-Huang Shih and Tun-Wen Pai*. Identification and Classification of Internal Repeats in Proteins  
P21. *Serghei Mangul and Alex Zelikovsky*. Haplotype Discovery from High-throughput Sequencing Data  
P22. *Atsushi Sasaki and Shinichi Morishita*. Robust Estimation of DNA Methylation with Local Regression  
P23. *Andrei Paun, Mihaela Paun, Alfonso Rodriguez-*

- Programming
- P6. *Pandurangan Sundaramurthy, Raashi Sreenivasan, Khader Shameer, Sunita Gakkhar and Ramanathan Sowdhamini.* HORIBALFRE: Higher Order Residue Interactions Based ALgorithm for Fold Recognition
- P7. *Simon Kocbek, Gregor Stiglic, Igor Pernek, Peter Kokol, Jun'ichi Tsujii, Rune Saetre, Jin-Dong Kim, Yoshimasa Tsuruoka and Sophia Ananiadou.* Analysis of Gene Ranking Algorithms with Extraction of Relevant Biomedical Concepts from Pubmed Publications
- P8. *Jing Hu, Marc Schilder and Xianghe Yan.* A Neighbor-Weighted K-Nearest Neighbor Method For Predicting Protein Subnuclear Localizations
- P9. *Venu Dasigi, Orlando Karam and Sailaja Pydimarri.* Issues in Functional Characterization and Clustering of Genes by Literature Mining
- P10. *William Valentine-Cooper, Yungui Huang, Sang-Cheol Seok and Veronica Vieland.* High-Performance Computing for Mapping
- P11. *Takanori Hasegawa, Rui Yamaguchi, Masao Nagasaki, Seiya Imoto and Satoru Miyano.* Comprehensive Pharmacogenomic Pathway Screening by Data Assimilation
- P12. *Yufeng Shen, Yiwei Gu and Itsik Pe'er.* A Hidden Markov Model for Copy Number Variant Prediction from Whole Genome Resequencing Data
- P13. *Nils Woetzel, Edward Lowe and Jens Meiler.* GPU-Accelerated Rigid Body Fitting of Atomic Structures into Electron Density Maps
- P14. *Edward Lowe, Nils Woetzel and Jens Meiler.* GPU-Accelerated Artificial Neural Network for QSAR Modeling
- P15. *Ankit Agrawal, Sanchit Misra, Ramanathan Narayanan, Lalith Polepeddi and Alok Choudhary.* A Lung Cancer Mortality Risk Calculator Based on SEER Data
- P16. *Paola Lecca, Ozan Kahramanogullari, Daniele Morpurgo, Corrado Priami and Ross Soo.* Modelling the Tumor Shrinkage Pharmacodynamics with BlenX
- P17. *Hongmei Chi and Peter Beerli.* Quasi-Monte Carlo Method in Population Genetics Parameter Estimation
- Paton and John Jack.* Biochemical Signaling: a Discrete Dimulation with Memory Enhancement
- P24. *Ham Ching Lam, Srinand Sreevatsan and Daniel Boley.* H3N2 Influenza Vaccine: A Historical Perspective
- P25. *Guozhen Liu, Han Zhang and George Quellinghorst.* Distinguishing Scientific Abbreviations and Genes in Bio-Medical Literature Mining
- P26. *Chiquito Crasto, Chandrahas Narne, Mikako Kawai, Landon Wilson and Stephen Barnes.* MRMPATH: A Web-based Tool that Identifies Peptide Transitions for LC-MRM-MS Analysis and its Application to Biological Pathways
- P27. *James Lindsay, Jin Zhang, Thomas Farnham, Edward Bullwinkel, Hamed Salooti, Ion Mandoiu, Yufeng Wu, Alex Zelikovsky and Rachel O'Neill.* Scaffolding Draft Genomes Using Paired Sequencing Data
- P28. *Marius Nicolae and Ion Mandoiu.* Empirical Comparison of Protocols for Sequencing-Based Gene and Isoform Expression Profiling
- P29. *Akshaye Dhawan and Alison Nolan.* Designing Reusable User-Interfaces for Browsing a Collection of Neuroscience Ontologies
- P30. *Sumit Kumar Jha and Christopher Langmead.* Synthesis of Biochemical Models Using Signatures
- P31. *Preetam Ghosh, Bhaswati Datta and Vijayraghavan Rangachari.* In Silico Hypotheses of the A42 Peptide Aggregation Process in Alzheimer's Disease
- P32. *Vijender Chaitankar, Preetam Ghosh, Mohamed Elasmri and Edward Perkins.* Gene Regulatory Network Inference Using Time Lagged Context Likelihood of Relatedness
- P33. *Ankit Agrawal, Sanchit Misra, Alok Choudhary and Karl Bilimoria.* Risk Prediction for Post-operative Adverse Outcomes in Colorectal Cancer Surgery
- P34. *Danhua Fan, Eric P. Rahrmann, Kevin A. T. Silverstein and David A. Largaespada.* Assessing the Content of Active Endogenous LINE1 Retrotransposons in Human Colorectal Cancer Samples Using High-throughput Pyrosequencing

5:30pm-  
7:00pm

Poster Session

# Friday, February 4, 2011

## 8:30am- Plenary Session

9:30am **Chair: Satoru Miyano**

Keynote talk: A Systems Biology Approach to Integrative Cancer Genomics  
*Andrea Califano* (Columbia University)

## 9:30am- Coffee Break

9:50am

## 9:50am- Parallel Sessions

11:50pm

### Session 4A: Invited talks

**Chair: Giri Narasimhan**

Invited talk: A Novel Perspective in Algorithmic Combinatorial Methods for Phasing Populations in a Coalescent Model

*Paola Bonizzoni* (University of Milano-Bicocca)

Invited talk: Reconciled Gene Trees and their Applications  
*Oliver Eulenstein* (Iowa State University)

Invited talk: Challenges in Metagenomic Assembly  
*Mihai Pop* (University of Maryland)

### Session 4B: CANGS Workshop

**Chair: Alex Zelikovsky**

*Rachel O'Neill*, The Utility of Next Generation Sequencing for Genome Scale Studies

*Dumitru Brinza*, Error Correction Methods in Next Generation Sequencing

*Srinivas Aluru*, Representative tiling for short read error correction

*Guocheng Yuan*, Targeting Mechanism of Epigenetic Factors

## 11:50pm- Lunch

1:10pm

## 1:10pm- Parallel Sessions

2:50pm

### Session 5A: Modeling

**Chair: Li-San Wang**

*Sumit Kumar Jha and Christopher Langmead*. Exploring Behaviors of SDE Models of Biological Systems using Change of Measures

*Saumyadipta Pyne, Hsiu J. Ho, Steven B. Haase and*

*Tsung-I Lin*. Parametric modeling of cellular state transitions as measured with flow cytometry

*Jun Chen, Peter Molnar and Aman Behal*. Maximum Likelihood Parameter Estimation in a Stochastic Resonate-and-Fire Neuronal Model

*Xu Wang, Sandip Roy and Yan Wan*. Using Deliberate-Delay Decentralized Controllers to Stop Spread Dynamics in Canonical Network Models

*Xiao Wu, Kathryn Sharpe, Ellen Li, Tianyi Zhang,*

*Hongyan Chen, Safiyh Taghavi, Daniel Van Der Lelie and Wei Zhu*. Comparative Genetic Pathway Analysis Using Structural Equation Modeling

### Session 5B: CANGS Workshop

**Chair: Rachel O'Neill**

*Mihai Pop*, Can you assemble whole genomes from next generation sequencing data?

*Jorge Duitama*, Bioinformatics Pipeline for Fosmid Based Molecular Haplotype Sequencing

*Irina Astrovskaya*, Inferring Viral Quasispecies from Ultra-Deep Sequencing Data

*Vamsi Kundeti*, Efficient Sequential and Parallel Algorithms for Processing Bi-directed de Bruijn Graphs

**2:50pm-  
3:10pm** Coffee Break

**3:10pm-  
5:30pm** Parallel Sessions

**Session 6A: High Performance Computing and Imaging**

**Chair: Sanguthevar Rajasekaran**

*Keith Bisset, Ashwin Aji, Madhav Marathe and Wuchun Feng.* High-Performance Biocomputing for Simulating the Spread of Contagion over Large Contact Networks

*Jian Zhang, Ian McQuillan and Fang-Xiang Wu.* Parallelizing Peptide-Spectrum Scoring Using Modern Graphics Processing Units

*Mayank Daga, Wuchun Feng and Thomas Scogland.* Towards Accelerating Molecular Modeling via Multi-Scale Approximation on a GPU

*Yuhong Zhang, Sanchit Misra, Daniel Honbo, Ankit Agrawal, Wei-keng Liao and Alok Choudhary.* Efficient Pairwise Statistical Significance Estimation for Local Sequence Alignment Using GPU

*Nathan Alexander, Nils Woetzel and Jens Meiler.* bcl::Cluster : A Method for Clustering Biological Molecules Coupled With Visualization in The Pymol Molecular Graphics System

*Yi Xiao, Tuan Pham, Jeff Chang and Xiaobo Zhou.* Symmetry-based Presentation for Stem-Cell Image Segmentation

*Martin Ehler, Jana Kainerstorfer, Zigurts Majumdar, Denise Cunningham, Mike Bono, Brian Brooks and Robert Bonner.* An Extended Curvature Correction Model for Clinical Optical Imaging

**Session 6B: CANGS Workshop**

**Chair: Ion Mandoiu**

*Wei Li,* Transcriptome Assembly from RNA-Seq Data: Objectives, Algorithms and Challenges

*John Karro,* Transcript Assembly Through a d2-based Minimum Spanning Tree approach

*Steffen Heber,* Using a Transcript Catalog and Paired-End RNA-Seq Data to Identify Differential Alternative Splicing

*Yufeng Shen,* Coverage Tradeoffs and Power Estimation in the Design of Whole-Genome Sequencing Experiments for Detecting Association

*Ben Raphael,* Characterization of Structural Variants with Next Generation DNA Sequencing

Closing roundtable discussion

**6:00pm-  
10:00pm** Banquet

# Saturday, February 5, 2011

## 8:30am- Plenary Session

9:30am Chair: *Teresa Przytycka*

Keynote talk: High-Resolution Sequence and Chromatin Signatures Predict Transcription Factor Binding in the Human Genome  
*Christina Leslie* (Memorial Sloan-Kettering Cancer Center)

## 9:30am- Coffee Break

9:50am

## 9:50am- Parallel Sessions

11:50am

**Session 7A: Data Mining and Phylogenetics**  
Chair: *Robert Aseltine*

Philippe Bordron, Damien Eveillard and Irena Rusu. SIPPER: A flexible method to integrate heterogeneous data into a metabolic network

Piotr Dittwald, Jerzy Ostrowski, Jakub Karczmariski and Anna Gambin. Inferring serum proteolytic activity from LC-MS/MS data

Ling Chen and Wei Liu. An Algorithm For Mining Frequent Patterns in Biological Sequence

D.K.Y. Chiu and P.S.C. Xu. InfoBarcoding: Selection of Non-contiguous Sites in Molecular Biomarker

George Mathew and Zoran Obradovic. A Privacy-preserving Framework for Distributed Clinical Decision Support

Louxin Zhang, Yen Kaow Ng, Taoyang Wu and Yu Zheng. Network Model and Efficient Method for Detecting Relative Duplications or Horizontal Gene Transfers

**Session 7B: Gene Structure and Expression Analysis**  
Chair: *Mihai Pop*

*Paola Bonizzoni, Gianluca Della Vedova, Yuri Pirola and Raffaella Rizzi.* PINtron: a Fast Method for Gene Structure Prediction via Maximal Pairings of a Pattern and a Text

*Patricia Buendia, Shu-Ning Hsu, Akira Chiba, John Tyree and Robert Lored.* From ESTs to ESRs: Comparative Analysis of Mutually Exclusive Exons in 15 Species of Insects

*Nirmalya Bandyopadhyay, Manas Somaiya, Tamer Kahveci and Sanjay Ranka.* Identifying Differentially Regulated Genes

*Amirali Jafarian and Alioune Ngom.* A New Gene Subset Selection Approach Based on Linearly Separating Gene Pairs

*Tianyi Zhang, Robert A. DeSimone, Hongyan Chen, Christina M Hamm, Jeffrey Yuan, Qing Qing Gong, Steven R.Hunt, Themistocles Dassopoulos, Rodney D. Newberry, Daniel N. Frank, Charles E. Robertson, Norman R.Pace, Erica Sodergren, George Weinstock, Xiangmin Jiao, Wei Zhu, Ellen Li.* Cluster Analysis of Genome-Wide Expression Differences in Disease-Unaffected Ileal Mucosa in Inflammatory Bowel Diseases

*Yinglei Lai.* The Analysis of Ordered Changes of Gene Expression and Gene-Gene Co-Expression Patterns

## 11:50am- Closing Remarks

12:00pm