# **ACM-BCB 2012**

The 2012 ACM International Conference on Bioinformatics, Computational Biology and Biomedicine









Association for Computing Machinery Orlando, Florida, USA October 7 – 10, 2012

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# Conference Schedule

Sunday Oct. 7	Monday Oct. 8	Tuesday Oct. 9	Wednesday Oct. 10
	8:45am – 9:00am Opening Remarks		
	9:00am– 10:00am Keynote Talk 1	9:00am– 10:00am Keynote Talk 2	9:00am–10:00am Keynote Talk 3
8:30am –6:30pm Workshop Sessions	10:00am – 10:30am Break	10:00am – 10:30am Break	10:00am-10:30am Break
	10:30am – Noon Three parallel paper sessions (1-3)	10:30am – Noon Three parallel paper sessions (10-12)	10:30am - Noon Three parallel paper sessions (19-21)
	Noon – 1:30pm Lunch	Noon – 1:30pm Lunch and Forum: Women in Bioinformatics	Noon – 1:30pm ACM-BCB 2012 Organization Committee Meeting
	1:30pm – 3:00pm Three parallel paper sessions (4-6)	1:30pm – 3:15pm Three parallel paper sessions (13-15)	1:30pm – 3:00pm Panel
	3:00pm – 3:30pm Break	3:15pm – 3:45pm Break	3:00pm – 4:00pm PhD Forum
3:15pm – 6:00pm Tutorials	3:30pm – 5:00pm Three parallel paper sessions (7-9)	3:45pm – 5:15pm Three parallel paper sessions (16-18)	
	5:00pm – 5:40pm ACM SIG Forum	6:30pm – 8:30pm Banquet	
	5:40pm – 7:00pm ACM SIG Organization Meeting		
	6:30pm – 8:30pm Poster session/Reception		

## Sunday, October 7, 2012

## Workshop 1: Immunoinformatics and Computational Immunology Workshop (ICIW 2012)

Location: San Juan 1

#### 8:30am – 10:30am Session I (Regular Talks)

- "Serum Antibody Repertoire Profiling Using Virtual Antigen Screen", Xinyue Liu, Luke Tallon, Lisa Sadzewicz, Elena Klyushnenkova and Yurij Ionov
- 2. "miHA-Match: computational detection of tissue-specific minor histocompatibility antigens", Magdalena Feldhahn, Pierre Dönnes, Benjamin Schubert, Karin Schilbach, Hans-Georg Rammensee and Oliver Kohlbacher
- "Decoding dendritic cell function through module and network analysis", Gaurav Pandey, Ariella Cohain, Jennifer Miller and Miriam Merad
- 4. "Using quantitative dose-response data to benchmark B-cell epitope prediction for antipeptide antibodies", Salvador Eugenio Caoili
- 5. "Immunoinformatic Analysis of Chinese Hamster Ovary (CHO) Protein Contaminants in Therapeutic Protein Formulations", Kristen Dasilva, Andres Gutierrez, Leonard Moise and Anne De Groot

#### 10:30am – 11:00am Morning Break

#### 11:00am - Noon Session II (Short Talks)

- "Human peptide homologues encoded by hepatitis C virus promote the response of regulatory T cells in chronically infected patients", Phyllis T. Losikoff, Loren D. Fast, Martha M. Nevola, Sasmita Mishra, Joe Desrosiers, William Martin, Matt Ardito, Frances Terry, Anne S. De Groot and Stephen H. Gregory
- "Minimal mutations that define lewis y reactive antibodies", Somdutta Saha, Anastas Pashov, Ramachandran Murali and Thomas Kieber-Emmons
- 3. "Human immunology project consortium (HIPC) database", Peter Li
- 4. "Quasi analysis of the HIV-1 Negative Regulatory Factor (Nef) sequences in the Los Alamos National Laboratory HIV sequence database: pattern and distribution of positive selection sites and their frequencies over years", Elnaz Shadabi Ma Luo, Rupert Capina, Binhua Liang and Francis Plummer
- "Immunogenicity scores across the Leishmania major proteome", Sebastian Loli, Andres H. Gutierrez, Mirko Zimic and Annie
  S. De Groot

#### Noon – 1:30pm Lunch

#### 1:30pm – 3:00pm Tutorial Part-I Immunoinformatics Resources

- 1. Introduction (15 minutes), Vasant Honavar
- 2. Immune Epitope Database (30 minutes), Bjoern Peters
- 3. Eukaryotic Pathogen Database Resources (30 minutes), Jessica Kissinger

#### 3:00pm – 3:30pm Afternoon Break

#### 3:30pm – 5:30pm Tutorial Part-II Immunoinformatics Tools

- 1. Predicting long MHC-I binders (30 minutes), Claus Lundegaard
- 2. iVAX: Interactive Vaccine Design Toolkit (45 minutes), Anne De Groot
- 3. Interactive Screening and Protein Re-engineering Interface (ISPRI) (45 minutes), Anne De Groot

#### 5:30pm – 6:30pm Poster Session

## Workshop 2: Biological Network Analysis and Applications in Translational and Personalized Medicine (BNA-M 2012)

#### Location: San Juan 2

#### 10:00am – Noon Session I (Regular Talks)

- "Genome Scale Inference of Transcriptional Regulatory Networks Using Mutual Information on Complex Interactions", Vijender Chaitankar, Preetam Ghosh, Mohamed O. Elasri, Kurt A. Gust and Edward J. Perkins
- 2. "Unraveling Multiple miRNA-mRNA Associations through a Graph based Approach", Pietro Hiram Guzzi, Pierangelo Veltri and Mario Cannataro
- "A Collective NMF Method for Detecting Protein Functional Module from Multiple Data Sources", Yuan Zhang, Nan Du, Liang Ge, Kebin Jia and Aidong Zhang

## Workshop 3: 1st International Workshop on Parallel and Cloud-based Bioinformatics and Biomedicine (ParBio 2012)

#### Location: San Juan 2

#### 1:00pm – 3:00pm Session I (Regular Talks)

- 1. "An Iterative MapReduce Approach to Frequent Subgraph Mining in Biological Datasets", Steven Hill, Bismita Srichandan and Rajshekhar Sunderraman
- 2. "High Performance Phosphorylation Site Assignment Algorithm for Mass Spectrometry Data Using Multicore Systems", Fahad Saeed, Trairak Pisitkun, Jason Hoffert and Mark Knepper
- "Parallelization of the Spectral Deconvolution Stage of the Proteomic Discovery Process", Neelam N. Deshpande and John A. Springer
- 4. "A System for Acquiring and Management of ECG Signals by Using Mobile Devices: a Support for First Intervention in Heart Attacks", Pietro Cinaglia, Giuseppe Tradigo, Pierangelo Veltri

## Workshop 4: 1st International Workshop on Robustness and Stability of Biological Systems and Computational Solutions

#### Location: San Juan 3

#### 1:00pm – 3:15pm

#### **Opening Remarks**

#### **Invited Talk**

"Robustness of problem-solving procedures in computational biology: A case study with the phylogenetic bootstrap", Bernard Moret

#### Session I (Regular Talks)

- 1. "Feature Extraction in Protein Sequences Classification: a New Stability Measure", Rabie Saidi, Sabeur Aridhi, Mondher Maddouri and Engelbert Mephu Nguifo
- "Robustness Measure for an Adeno-Associated Viral Shell Self-Assembly Is Accurately Predicted by Configuration Space Atlasing Using EASAL", Ruijin Wu, Aysegul Ozkan, Antonette Bennett, Mavis Agbandje-Mckenna and Meera Sitharam
- 3. "A Monte Carlo Approach to Measure the Robustness of Boolean Networks", Vitor H. P. Louzada, Fabricio M. Lopes, Ronaldo F. Hashimoto

#### **Contributed Talk**

"Stability in Computational Biology: Current and Future Applications", Saad Sheikh

## Tutorials

### **Tutorial 1**

#### 3:15pm-5:15pm Location: San Juan 2

## Title: An Introduction to Evolutionary Computation for Bioinformatics

## Clare Bates Congdon, University in Southern Maine

**Abstract:** Evolutionary Computation (EC) is a powerful search method inspired by natural evolution. In EC, candidate solutions exist in a population, and new candidate solutions are generated from existing solutions using operators such as recombination and mutation. With a selection pressure that favors the better solution, over a number of generations, the population tends to include better and better solutions to the task.

This tutorial will introduce the audience to EC and to several example applications of EC to Bioinformatics research. Example applications include sequence analysis, phylogenetics, and classification/data mining.

## **Tutorial 2**

### 3:15pm-6:00pm

#### Location: San Juan 3

## Title: A survey of Computational Approaches to reconstruct, Partition, and Query Biological Networks

### Thair Judeh and Dongxiao Zhu, Wayne State University

**Abstract:** By reconstructing, partitioning, and querying biological networks, various biological insights may be gained. Using high-throughput data such as gene expression data or unstructured gene sets, network reconstruction may provide a more systematic view of the underlying biological condition. It may, however, only be a first step in the analysis. In particular, network partitioning is important as it allows for the extraction of subnetworks that may serve as functional units of the underlying condition. Furthermore, many biological network databases are currently available. Via network querying, researchers are able to query their hypotheses against these databases. Thus, having a solid understanding of reconstructing, partitioning, and querying biological networks can be a great asset for bioinformatics research.

## Monday, October 8, 2012

## **Opening Remarks**

8:45am – 9:00am Location: San Juan Ballroom

## Keynote Talk 1

9:00am – 10:00am Session Chair: Aidong Zhang Location: San Juan Ballroom

## Title: Genomic Location is Information: Towards Understanding the Organizational Principles of Bacterial Genomes

### Ying Xu, University of Georgia, Athens

**Abstract:** We have recently discovered that genomic locations of genes in bacteria are highly constrained by the cellular processes that are involved in. So for the first time, we understand that the locations of genes follow both global and local rules. This realization has led to a new paradigm for tackling and solving some very challenging genomic analysis problems. I will discuss about this new discovery and a number of applications that we are currently doing, including gene assignments of pathway holes and complete genome assembly.

10:00am – 10:30am Morning Break

## **Paper Sessions**

#### 10:30am – Noon

#### Session 1 Systems Biology Session Chair: Mehmet Koyuturk Location: San Juan 1

Session 2 Protein and RNA Structure (Short Presentations) Session Chair: Chris Bystroff Location: San Juan 2

- "STEROID: In Silico Heuristic Target Combination Identification for Disease-Related Signaling Networks", Huey Eng Chua, Sourav S Bhowmick, Lisa Tucker-Kellogg and C Forbes Dewey Jr
- "Functional Module Identification by Block Modeling using Simulated Annealing with Path Relinking", Yijie Wang and Xiaoning Qian
- "Complexity reduction of Stochastic Master Equation Simulation based on Kronecker Product Analysis", Mehmet Umut Caglar and Ranadip Pal

- "Memory-Based Local Search for Simplified Protein Structure Prediction", Swakkhar Shatabda, M.A.Hakim Newton, Duc Nghia Pham and Abdul Sattar (S)
- "Towards Biophysical Validation of Constraint Modeling for Rigidity Analysis of Proteins", Filip Jagodzinski and Ileana Streinu (S)
- "Predicting Protective Bacterial Antigens Using Random Forest Classifiers", Yasser El-Manzalawy, Drena Dobbs and Vasant Honavar (S)
- "Simulation and Analysis of Antibody Aggregation on Cell Surfaces Using Motion Planning and Graph Analysis", Kasra Manavi, Bridget Wilson and Lydia Tapia (S)
- "Building the Initial Chain of the Proteins through De Novo Modeling of the Cryo-Electron Microscopy Volume Data at the Medium Resolutions", Kamal Al Nasr, Lin Chen, Dong Si, Desh Ranjan, Muhammad Zubair and Jing He (S)

#### Session 3 Invited Talks Session Chair: Chris Bailey-Kellogg Location: San Juan 3

- "Probabilistic Search Frameworks for Modeling Structures and Motions of Protein Systems", Amarda Shehu
- "ProteinHistorian: Tools for the Comparative Analysis of Eukaryote Protein Origin", John Capra
- "SMURFLite: combining simplified Markov random fields with simulated evolution improves remote homology detection for beta-structural proteins into the twilight zone", Lenore Cowen (S)

## Noon – 1:30pm Lunch (Lunch will NOT be provided)

#### Session 4 Comparative Genomics, Population & Cancer Genomics Session Chair: Oliver Eulenstein Location: San Juan 1

- "Coalescent-based Method for Learning Parameters of Admixture Events from Large-Scale Genetic Variation Data", Ming-Chi Tsai, Guy Blelloch, R Ravi and Russell Schwartz
- "Inferring Ancestry in Admixed Populations using Microarray Probe Intensities", Chen-Ping Fu, Catherine E. Welsh, Fernando Pardo-Manuel de Villena and Leonard McMillan
- "Algorithms for Detecting Complementary SNPs within a Region of Interest That Are Associated with Diseases", Sinan Erten, Marzieh Ayati, Yu Liu, Mark R. Chance and Mehmet Koyuturk

Session 5 Algorithms for Sequence Analysis (Short Presentations) Session Chair: Ferhat Ay Location: San Juan 2

1:30pm – 3:00pm

- "Parallel Syntenic Alignment on GPUs", Junjie Li, Sanjay Ranka and Sartaj Sahni (S)
- "An Integer Programming Approach to Novel Transcript Reconstruction from Paired-End RNA-Seq Reads", Serghei Mangul, Adrian Caciula, Sahar Al Seesi, Dumitru Brinza, Abdul Rouf Banday, Rahul N. Kanadia, Ion Mandoiu and Alex Zelikovsky (S)
- "A fast computation of pairwise sequence alignment scores between a protein and a set of variants of another protein", Yongwook Choi (S)
- "Scalable Genome Scaffolding using Integer Linear Programming", James Lindsay, Hamed Salooti, Alex Zelikovsky and Ion Mandoiu (S)
- "Alignment seeding strategies using contiguous pyrimidine purine matches", Minmei Hou, Louxin Zhang and Robert Harris (S)

#### Session 6 Invited Talks Session Chair: Wei Wang Location: San Juan 3

- "Optimization algorithms for the design of immunotolerant biotherapies", Chris Bailey-Kellogg
- "Deriving protein statistical potential using the Boltzmann law and machine learning", Jinbo Xu
- "Biological Interpretation of Morphological Patterns in Histopathological Whole-Slide Images", Sonal Kothari, John H. Phan, Adeboye O. Osunkoya and May D. Wang

### 3:00pm – 3:30pm Afternoon Break

### 3:30pm – 5:00pm

Session 7 Protein and RNA Structure Session Chair: Lenore Cowen Location: San Juan 1 Session 8 Systems Biology (Short Presentations) Session Chair: Xiaoning Qian Location: San Juan 2

- "A Multi-Directional Rapidly Exploring Random Graph (mRRG) for Protein Folding", Shuvra Kanti Nath, Shawna Thomas, Chinwe Ekenna and Nancy M. Amato
- "Biased Decoy Sampling to Aid the Selection of Near-native Protein Conformations", Kevin Molloy and Amarda Shehu
- "Exploring objective functions and cross-terms in the optimization of an energy function for protein design", Yao-Ming Huang and Chris Bystroff

- "Efficient Implementation of the Hybrid Method for Stochastic Simulation of Biochemical Systems", Shuo Wang and Yang Cao (S)
- "Network-based classification of recurrent endometrial cancers using high-throughput DNA methylation data", Jianhua Ruan, Md. Jamiul Jahid, Fei Gu, Chengwei Lei, Yi-Wen Huang, Ya-Ting Hsu, David G. Mutch, Chun-Liang Chen, Nameer B. Kirma and Tim H. Huang (S)
- "ADANET: Inferring Gene Regulatory Networks using Ensemble Classifiers", Janusz Slawek and Tomasz Arodz (S)
- "Microarray vs. RNA-Seq: A comparison for active subnetwork discovery", Ayat Hatem, Kamer Kaya and Ümit V. Çatalyürek (S)
- "QSEA for fuzzy subgraph querying of KEGG pathways", Thair Judeh, Tin Chi Nguyen and Dongxiao Zhu (S)

#### Session 9 Invited Talks Session Chair: Wei Wang Location: San Juan 3

- "Non-overlapping clone pooling for high-throughput sequencing", Reginaldo Kuroshu
- "Discovering Geometric Patterns in Genomic Data", Wenxuan Gao, Christopher Brown, Robert L. Grossman, Lijia Ma, Matthew Slattery, Kevin P. White, Philip S. Yu
- "PseudoDomain: identification of processed pseudogenes based on protein domain classification", Yuan Zhang and Yanni Sun

## ACM SIG Forum Session

5:00pm-5:40pm Location: San Juan 1

# ACM SIG Organization Meeting

5:40pm-7:00pm Location: Eola Ballroom

# Poster Session/Reception

6:30pm-8:30pm Location: San Juan Ballroom

List of accepted posters are at the end of this brochure

## Tuesday, October 9, 2012

## Keynote Talk 2

9:00am – 10:00am Session Chair: Tamer Kahveci Location: San Juan Ballroom

### **Title: Transcription Factors and DNA Regulatory Elements**

#### Martha L. Bulyk, Brigham & Women's Hospital and Harvard Medical School

**Abstract:** The interactions between sequence-specific transcription factors (TFs) and their DNA binding sites are an integral part of the gene regulatory networks within cells. My group developed highly parallel in vitro microarray technology, termed protein binding microarrays (PBMs), for the characterization of the sequence specificities of DNA-protein interactions at high resolution. Using PBMs, we have determined the DNA binding specificities of hundreds of TFs from a wide range of species. More recently we have used the PBM technology to investigate TF heterodimers and higher order complexes. The PBM data have permitted us to identify novel TFs and their DNA binding sequence preferences, predict the target genes and condition-specific regulatory roles of TFs, predict and analyze tissue-specific transcriptional enhancers, investigate functional divergence of paralogous TFs within a TF family, investigate the molecular determinants of TF-DNA recognition specificity, and distinguish direct versus indirect TF-DNA interactions in vivo. Notably, not all DNA binding sites of a TF function equally. Further analyses of TFs and cis regulatory elements are likely to reveal features of cis regulatory sequences that are important in gene regulation.

10:00am – 10:30am Morning Break

## **Paper Sessions**

#### 10:30am – Noon

#### Session 10 Systems Biology Session Chair: Jinbo Xu Location: San Juan 1

Session 11 Comparative Genomics, Population & Cancer Genomics (Short Presentations) Session Chair: Rui Kuang Location: San Juan 2

- "NetPipe: A Network-based Pipeline for Discovery of Genes and Protein Complexes Regulating Meiotic Recombination Hotspots", Min Wu, Chee Keong Kwoh, Xiaoli Li and Jie Zheng
- "Reverse Engineering Molecular Hypergraphs", Ahsanur Rahman, Christopher L. Poirel, David J. Badger and T. M. Murali
- "Supervised Logistic Principal Component Analysis for Pathway Based Genome-Wide Association Studies", Meng Lu, Jianhua Huang and Xiaoning Qian

- "Finding Informative Genes for Prostate Cancer: A General Framework of Integrating Heterogeneous Sources", Liang Ge, Jing Gao, Nan Du and Aidong Zhang (S)
- "Integration of Genomic and Epigenomic Features to Predict Meiotic Recombination Hotspots in Human and Mouse", Min Wu, Chee Keong Kwoh, Teresa M. Przytycka, Jing Li and Jie Zheng (S)
- "Inferring novel associations between SNP sets and gene sets in eQTL study using sparse graphical model", Wei Cheng, Xiang Zhang, Yubao Wu, Xiaolin Yin, Jing Li, David Heckerman and Wei Wang (S)
- "A pattern mining based integrative framework for biomarker discovery", Sanjoy Dey, Gowtham Atluri, Michael Steinbach, Kelvin Lim, Angus MacDonald and Vipin Kumar (S)

#### Session 12 Protein and RNA Structure and Invited Talk Session Chair: Ileana Streinu Location: San Juan 3

- "Protein Structure and Sequence Mining for Improving Computational Design of Stable Proteins", Jianwen Fang
- "Protein Blocks Versus Hydrogen Bonds Based Alphabets For Protein Structure Classification", Dino Franklin
- "ArtSurf: A Method for Deformable Partial Matching of Protein Small-Molecule Binding Sites", Jeffrey Van Voorst, Yiying Tong and Leslie Kuhn

 "SNPRank: An Efficient Ranking Method for Genome-wide Association Studies", Jie Liu, Humberto Vidaillet, Elizabeth Burnside and David Page (S)

## Noon – 1:30pm Lunch (Lunch will be provided by the conference)

## Forum: Women in Bioinformatics

Noon-1:30pm Location: Eola Ballroom Session Co-Chairs: Wei Wang, UCLA and May Wang, Georgia Tech

## **Paper Sessions**

### 1:30pm – 3:15pm

#### Session 13 Protein and RNA Session Chair: Brian Chen Location: San Juan 1

- "Multi-target protein-chemical interaction prediction using taskregularized and boosted multi-task learning", Jintao Zhang, Gerald Lushington and Jun Huan
- "Functional Site Prediction by Exploiting Correlations between Labels of Interacting Residues", Saradindu Kar, Deepak Vijayakeerthi, Balaraman Ravindran

- Session 14 Systems Biology and Contributed Presentation Session Chair: Amarda Shehu Location: San Juan 2
- "Three differentiation states riskstratify bladder cancer into distinct subtypes", Jens-Peter Volkmer, Debashis Sahoo, Robert Chin, Philip Ho, Chad Tang, Antonina Kurtova, Stephen Willingham, Senthil Pazhanisamy, Humberto Contreras-Trujillo, Theresa Storm, Yair Lotan, Andrew Beck, Benjamin Chung,

Session 15 Text Mining and Contributed Presentations Session Chair: Tamer Kahveci Location: San Juan 3

- "Protein Function Prediction using Text-based Features extracted from Biomedical Literature: The CAFA Challenge", Andrew Wong and Hagit Shatkay
- "Anaphora Resolution in Biomedical Literature: A Hybrid Approach", Jennifer D'Souza and Vincent Ng

and Ashish V. Tendulkar

 "A Volumetric Method for Representing and Comparing Regions of Electrostatic Focusing in Molecular Structure", Brian Chen and Debdas Paul Ash Alizadeh, Guilherme Godoy, Seth Lerner, Matt van de Rijn, Linda Shortliffe, Irving Weissman and Keith Chan

- "Evolutionary Analysis of Functional Modules in Dynamic PPI Networks", Nan Du, Yuan Zhang, Kang Li, Jing Gao and Aidong Zhang
- "Predicting expression-related features of chromosomal domain organization with networkstructured analysis of gene expression and chromosomal location", Vinodh Rajapakse, Wojciech Czaja, William Reinhold, Yves Pommier and Sudhir Varma
- "Remote Homology Detection on Alpha-Structural Proteins Using Simulated Evolution", Mengfei Cao and Lenore Cowen

#### 3:15pm – 3:45pm Afternoon Break

- "OCR-based Image Features for Biomedical Image and Article Classification: Identifying Documents relevant to Cis-Regulatory Elements", Hagit Shatkay, Ramya Narayanaswamy, Santosh Nagaral, Na Harrington, Rohith Mv, Gowri Somanath, Ryan Tarpine, Kyle Schutter, Tim Johnstone, Dorothea Blostein, Sorin Istrail and Chandra Kambahmettu
- "Hybrid pattern matching for complex ontology term recognition", Jung-Jae Kim and Luu Anh Tuan (S)

## 3:45pm – 5:15pm

Session 16 Algorithms for Sequence Analysis Session Chair: Tony Capra Location: San Juan 1

 "Efficient SNP-sensitive alignment and database-assisted SNP calling for low coverage samples", Ruibang Luo, Chi Man Liu, Thomas Wong, Chang Yu, Tak-Wah Lam, Siu Session 17 Modeling, Querying and Systems Biology Session Chair: Hagit Shatkay Location: San Juan 2

 "3D Bone Microarchitecture Modeling and Fracture Risk Prediction", Hui Li, Xiaoyi Li, Lawrence Bone, Cathy Buyea, Murali Ramanathan and Aidong Session 18 Invited Talks Session Chair: Ümit V. Çatalyürek Location: San Juan 3

 "Assessing and Improving the Reliability of Short Read Alignments for Next Generation Sequencing", Mehmet Koyuturk Ming Yiu, Ruiqiang Li and Hingfung Ting

- "ERNE-BS5: aligning BS-treated sequences by multiple hits on a 5letters alphabet", Nicola Prezza, Cristian Del Fabbro, Francesco Vezzi, Emanuele De Paoli and Alberto Policriti
- "Improved Multiple Sequence Alignments using Coupled Pattern Mining", K. S. M. Tozammel Hossain, Debprakash Patnaik, Srivatsan Laxman, Prateek Jain, Chris Bailey-Kellogg and Naren Ramakrishnan

#### Zhang (S)

- "Semantic Querying over Knowledge in Biomedical Text Corpora Annotated with Multiple Ontologies", Watson Wei Khong Chua and Jung-Jae Kim (S)
- "Parallel Verlet Neighbor List Algorithm for GPU-Optimized MD Simulations", Tyson Lipscomb, Anqi Zou and Samuel Cho (S)
- "Signed Network Propagation for Detecting Differential Gene Expressions and DNA Copy Number Variations", Wei Zhang, Nicholas Johnson, Baolin Wu and Rui Kuang (S)

- "Mining Genetic Interactions in Genome-Wide Association Study", Wei Wang
- "Supertrees and Supertree Problems", Oliver Eulenstein

**6:30pm – 8:30pm Banquet** Location: San Juan Ballroom

## Wednesday, October 10, 2012

## Keynote Talk 3

9:00am – 10:00am Session Chair: Mona Singh Location: San Juan Ballroom

#### **Title: Machine Learning Approaches in Proteomics**

### Pierre Baldi from the University of California, Irvine (UCI)

Abstract: Over the past three decades machine learning approaches have had a profound influence on many fields, including bioinformatics. We will provide a brief historical perspective of machine learning and its applications to proteomics, particularly structural proteomics, and discuss why structural proteomics is important for machine learning. We will then present state-of-the art machine learning methods for predicting protein structures and structural features, from secondary structure to contact maps. We will stress and demonstrate the importance of combining supervised and unsupervised learning, and using deep and modular architectures capable of integrating information over space and "time" at multiple scales. Finally, we will describe two proteomic applications that have benefited from statistical machine learning methods: (1) the discovery of new drug leads for neglected diseases; and (2) the development of high-throughput platforms to study the immune response with applications to antigen discovery and vaccine development.

10:00am – 10:30am Morning Break

## **Paper Sessions**

#### 10:30am – Noon

#### Session 19 Databases, Knowledgebases & Ontologies Session Chair: Jing Gao Location: San Juan 1

Session 20 Algorithms for Sequence Analysis (Short Presentations) Session Chair: Ion Mandoiu Location: San Juan 2

#### Session 21 Bioimage Analysis Session Chair: May D. Wang Location: San Juan 3

- "What We Found on Our Way to Building a Classifier: A Critical Analysis of the Screening Questionnaire for Young Athletes", Hagit Shatkay
- "Protein Function Prediction using Weak-label Learning", Guoxian Yu, Guoji Zhang, Huzefa Rangwala, Carlotta Domeniconi and Zhiwen Yu
- "Detecting ECG Abnormalities via Transductive Transfer Learning", Kang Li, Nan Du and Aidong Zhang

- "A New Algorithm for Finding Enriched Regions in ChIP-Seq Data", Iman Rezaeian and Luis Rueda (S)
- "DACIDR: Deterministic Annealed Clustering with Interpolative Dimension Reduction using Large Collection of 16S rRNA Sequences", Yang Ruan, Saliya Ekanayake, Mina Rho, Haixu Tang, Seung-Hee Bae, Judy Qiu and Geoffrey C. Fox (S)
- "An integrated optimization framework for inferring twogeneration kinships and parental genotypes from microsatellite samples", Daehan Won, Chun-An Chou, W. Art Chaovalitwongse, Tanya Y. Berger-Wolf, Bhaskar Dasgupta, Ashfaq A. Khokhar, Marco Maggioni, Mary V. Ashley, Jason Palagi and Saad Sheikh (S)
- "On enumerating the DNA sequences", M. Oguzhan Kulekci (S)
- "Rational design of Orthogonal Libraries of Protein Coding Genes",

- "Automatic Segmentation and Quantification of Filamentous Structures in Electron Tomography", Leandro Loss, Hang Chang, Purbasha Sarkar, Manfred Auer and Bahram Parvin
- "Multivariate Hypergeometric Similarity Measure", Chanchala Kaddi, R. Mitchell Parry and May D. Wang
- "Alignment of Real-Time Live-Cell Growth Data for Quantitative Analysis of Growth at the Shoot Apex of Arabidopsis thaliana", Oben M Tataw, G.V. Reddy and A. K. Row-Chowdhurry

Daniel Ryan and Dimitris

Papamichail (S)

### Noon – 1:30pm ACM-BCB 2012 Organization Committee Meeting Location: Eola Ballroom

## Panel

1:30pm-3:00pm Location: San Juan Ballroom

## Panel topic: Bigdata in Biosciences: Challenges and Opportunities Panel chair: Srinivas Aluru, Iowa State University

#### Panelists

Ümit V. Çatalyürek, Ohio State University Alin Dobra, University of Florida Vasant Honavar, National Science Foundation Ion Mandoiu, University of Connecticut Bernard Moret, École Polytechnique Fédérale de Lausanne

## **PHD** Forum

3:00pm-4:00pm Location: San Juan Ballroom

### Chair: Rahul Singh, San Francisco State University

#### **List of Attendees**

Sanjoy Dey Ming-Chi Tsai Ahsanur Rahman Chanchala Kaddi Vishakha Sharma Shuo Wang Yuan Zhang Meng Lu Ayat Ahmed Hatem Yijie Wang Jie Liu Wei Zhang Wei Cheng Chen-ping Fu Mehmet Umut Caglar Bismita Srichandan Guoxian Yu Serghei Mangul Junjie Li Mengfei Cao Thair Judeh Wenxuan Gao Kang Li

## **List of Accepted Posters**

"A Novel Approach for Mining Representative Spatial Motifs of Proteins", Wajdi Dhifli, Rabie Saidi and Engelbert Mephu Nguifo

"Systems Biology Approach to Identify Markers of Differentiation in Bladder Cancer", Debashis Sahoo, Jens-Peter Volkmer, Robert Chin, Philip Ho, Chad Tang, Antonina Kurtova, Stephen Willingham, Senthil Pazhanisamy, Humberto Contreras-Trujillo, Theresa Storm, Yair Lotan, Andrew Beck, Benjamin Chung, Ash Alizadeh, Guilherme Godoy, Seth Lerner, Matt van de Rijn, Linda Shortliffe, Irving Weissman, Keith Chan

"454 and SOLiD Complementary Used to Filter and Build the Draft Genome of Highly Abundant Cyanobacteria in Biological Desert Crust", Yoram Shotland

"An In-depth Analysis of the Molecular Dynamics and Structural Aspects of IKB Proteins", Shaherin Basith and Sangdun Choi

"mHMM (multivariate Hidden Markov Model) Application in Studying BRD4 and JMJD6 Function Cooperatively on Promoter-proximal Polymerase-II (Pol II) Pausing Release", Qi Ma, Wen Liu and Michael G Rosenfeld

"Phylogenetic and Functional Divergence Analysis of Vertebrate IRAK Family Members", Vijayakumar Gosu and Sangdun Choi

"Multi-level Structural Domain-domain Interactions for Prediction of Obligate and Non-obligate Protein-protein Interactions", Michael Hall, Mina Maleki and Luis Rueda

"Identification of Protein Stability Patches that Pinpoint Key Structural or Functional Sites", Marie De Laet, Yves Dehouck, Dimitri Gilis, Marianne Rooman

"Searching for the Relics of Primitive Codons", Satoshi Mizuta and Taro Mori

"Efficient SDH Computation in Molecular Simulations Data", Yi-Cheng Tu, Shaoping Chen, Sagar Pandit, Anand Kumar and Vladimir Grupcev

"A Computational Metabolic Model of the NG108-15 Cell for High Content Drug Screening with Electrophysiological Readout", Aditya Reddy Kolli, Frank Sommerhage, Peter Molnar, Jonathan Hood, Jerry Jenkins, Faraz Hussain, Arup K. Ghosh, Sumit Kumar Jha and James Hickman "A Novel Mathematical Basis for Predicting Somatic Single Nucleotide Variants from Next-generation Sequencing", Eric Bareke, Jean-Francois Spinella, Ramon Vidal, Jasmine Healy, Daniel Sinnett and Miklos Csuros

"Nuclear Localization Signal Prediction Based on Sequential Pattern Mining", Jhih-Rong Lin and Jianjun Hu

"Pattern Analysis: a Web-based Tool for Analyzing Response Patterns in Low-replication, Many-treatment Gene Expression Data", Nam S. Vo and Vinhthuy Phan

"ngALL Database : A Flexible Framework for the Management and Integration of Childhood Leukemia Next Generation Sequencing data", Pascal St-Onge, Virginie Saillour, Patrick Beaulieu, Robert Hamon, Jasmine Healy and Daniel Sinnett

"Secondary Structure Predictions for Long RNA Sequences Based on Inversion Excursions-Preliminary Results", Daniel T. Yehdego, Vikram Kumar Reddy Kodimala, Sameera Viswakula, Boyu Zhang, Rahulsimham Vegesna, Kyle L. Johnson, Michela Taufer and Ming-Ying Leung

"Rapid Efficient Macromolecular Substructure Searching in a Cloud", Jeffrey Van Voorst and Barry Finzel

"Classification of Multicolor Fluorescence In-Situ Hybridization (M-FISH) Image Using Regularized Multinomial Logistic Regression", Jingyao Li, Hongbao Cao, Yu-Ping Wang

"Copy Number Variation Estimation from Multiple Nextgeneration Sequencing Samples", Junbo Duan, Ji-Gang Zhang; Hongbao Cao, Hong-Wen Deng; Yu-Ping Wang

"Entropy-based Evaluation Function for the Investigation of Genetic Code Adaptability", Lariza Laura de Oliveira and Renato Tinos

"Shortest Paths Ranking Methodology to Identify Alterations in PPI Networks of Complex Diseases", Sergio Nery Simoes, David Correa Martins Jr, Helena Brentani and Ronaldo Fumio Hashimoto

"Prediction of Candidate Genes for Neuropsychiatric Disorders Using Feature-based Enrichment", Bingqing Xie, Dinanath Sulakhe, Bhadrachalam Chitturi, Gady Agam, Natalia Maltsev and T. Conrad Gilliam "A Graph-based Cluster Ensemble Method to Detect Protein Functional Modules from Multiple Information Sources", Yuan Zhang, Liang Ge, Nan Du, Guoqiang Fan, Kebin Jia and Aidong Zhang

"Macromolecular Modeling of Protein Structure - SCI1 of Nicotiana tabacum L.", Marcelo Filipe Breda de Moraes, Nilson Nicolau Junior and Silvana Giuliatti

"A Continuum Hard-Sphere Model of Protein Adsorption", Craig Finch and James Hickman

"Genecentric: A Package to Uncover Graph-theoretic Structure in High-throughput Epistasis Data", Andrew Gallant, Mark D.M. Leiserson, Maxim Kachalov, Lenore J. Cowen and Benjamin J. Hescott

"Predicting Possible Directed-graph Patterns of Gene Expressions in Studies Involving Multiple Treatments", Nam S. Vo, Vinhthuy Phan and Thomas Sutter

"A Brief Comparison of DSP and HMM Methods for Gene Finding", Sajid A. Marhon and Stefan C. Kremer

"Computational Tool for the Automated Large-Scale GPIomic Analysis", Clemente Aguilar-Bonavides, Ming-Ying Leung, Ernesto S. Nakayasu, Felipe Gazos-Lopes and Igor C. Almeida

"A Machine-learning Approach to Retrieving Diabetic Retinopathy Images", Parag S. Chandakkar, Ragav Venkatesan, Baoxin Li and Helen K. Li

"An Evolutionary Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space", Brian Olson and Amarda Shehu

"Empirical Metabolite Identification via GA Feature Selection and Bayes Classification", Paul Anderson and Michael Peterson

"A Next Generation Sequence Processing and Analysis Platform with Integrated Cloud-storage and High Performance Computing Resources", Jeremy C. Morgan, Robert W. Chapman and Paul E. Anderson

"gLIMS: Google Cloud-based Laboratory Information Management System for NMR Metabolomics", Edward Pharr, Aspen Olmsted and Paul E. Anderson "A Comparative Study of cCodon Adaptation in ssDNA and dsDNA Phages", Shivapriya Chithambaram, Ramanandan Prabhakaran and Xuhua Xia

"RNA-DV: an Interactive Tool for Editing and Visualizing RNA Secondary Structures", Herbert H. Tsang and Denny C. Dai

"Robust Differential Co-Expression Discovery: an Insight into Pharmacodynamics of Tyrosine Kinase Inhibitor", Xi Gao and Tomasz Arodz

"Towards Sequence-Based DNA Flexibility Analysis", Emily Flynn, Filip Jagodzinski and Ileana Streinu

"Simulation and Study of Large-Scale Bacteria-Materials Interactions via BioScape Enabled by GPUs", Jie Li, Vishakha Sharma, Narayan Ganesan and Adriana Compagnoni

"How to Select Microscopy Image Similarity Metrics?", Peter Bajcsy, Joe Chalfoun and Mary Brady

"Approximate Subspace Pattern Mining for Mapping Copy-Number Variations", Nicholas Johnson, Gang Fang and Rui Kuang

"Microbial Source Tracking by Molecular Fingerprinting", Jan Lorenz Soliman, Aldrin Montana, Kevin Webb, Alex Dekhtyar, Michael Black, Chris Kitts, Jennifer Vanderkellen, Emily Neal, Anya Goodman

"Random-Walk: a Stagnation Recovery Technique for Simplified Protein Structure Prediction", Mahmood A Rashid, Swakkhar Shatabda, M.A.Hakim Newton, Md Tamjidul Hoque, Duc Nghia Pham and Abdul Sattar

"Empirical Bayesian LASSO for Pathway-Based Genome Wide Association Studies", Xiaodong Cai

"Web-enabled systems biology Science gateway on supercomputers", Bhanu Rekepalli, Paul Giblock, Christopher Reardon, Subhra Sarkar and Mark Fahey

"Assigning statistical confidence estimates to DNA-DNA interactions from genome-wide chromosome conformation capture assays", Ferhat Ay, Timothy L. Bailey and William S. Noble

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## Notes

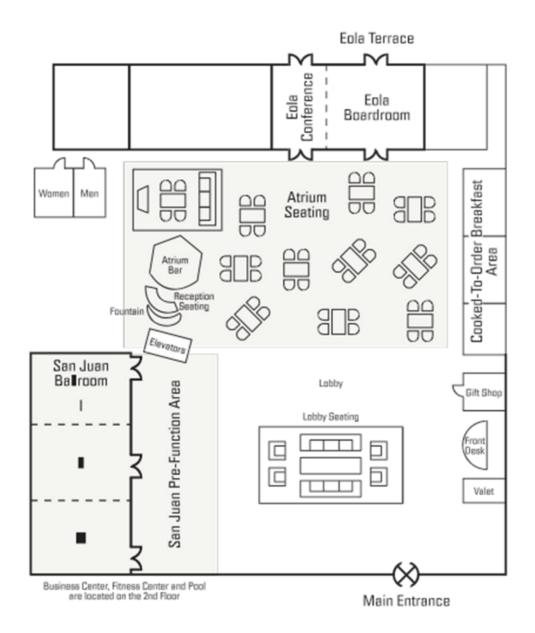
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# Notes

## Embassy Suites Orlando Downtown Floor Plan



## Message from the General Chair

It is my great pleasure to welcome you to ACM BCB 2012. ACM BCB has established itself as a premier annual forum for research and development in Bioinformatics, Computational Biology and Biomedicine from academia, industry and government. The conference focuses on interdisciplinary and multidisciplinary research in disciplines of computer science, mathematics, statistics, biology, bioinformatics, and biomedicine. This year's conference received 159 papers. After a rigorous review process, 33 regular papers and 31 short papers were selected. The conference program also has 9 invited papers, 3 contributed papers and 43 poster papers. The program features three keynote speeches, two tutorials and the following four workshops:

- 1. Immunoinformatics and Computational Immunology Workshop
- 2. Biological Network Analysis and Applications in Translational and Personalized Medicine
- 3. Parallel and Cloud-based Bioinformatics and Biomedicine
- 4. Robustness and Stability of Biological Systems and Computational Solutions

The best paper, best student paper and best poster will be selected during the conference. The selection will be announced during the banquet. The success of this conference has been due to the significant time commitment and diligent effort of many individuals. In particular, Tamer Kahveci and Mona Singh, with their track chairs and the members of the Program Committee, have been pivotal in spearheading the review process and selecting an excellent set of research papers. Vasant Honavar was responsible for four high quality workshops; Srinivas Aluru for organizing the panel; and Ümit V. Çatalyürek and Kamer Kaya for organizing the poster session. I would like to take this opportunity to extend our thanks to all of them as well as workshop organizers that have helped in putting together a very strong technical program.

Special thanks also go to Hu Haiyan, Xiaoning Qian, Sumit Jha and Arup Ghosh for local arrangements; Jing Li for tutorials; Mehmet Koyuturk for publicity; Rahul Singh for PHD Forum; Preetam Ghosh for registrations; Jing Gao for managing the proceedings; and Kang Li for managing the website.

I would also like to thank Aidong Zhang, chair of the steering committee, and the members of the steering committee for their unwavering support. Aidong was always available to provide feedback and her help was invaluable. I would like to thank the National Science Foundation (NSF) for travel support of graduate students. The NSF support allows the students with opportunities to interact with the distinguished speakers, to present their own research ideas, and to foster new collaborations. On behalf of the organizing committee, I appreciate your participation and welcome you to Orlando, Florida! Hope you enjoy the conference.

Sanjay Ranka General Chair ACM-BCB 2012