

2013 ACM Conference on Bioinformatics, Computational Biology and Biomedical Informatics

ACM - BCB 2013



Washington, D.C., U.S.A.
September 22 - 25, 2013



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Conference Schedule

Sunday Sep. 22	Monday Sep. 23	Tuesday Sep. 24	Wednesday Sep. 25
	8:15am – 8:30am Opening Remarks		
	8:30am – 9:30am Keynote Talk 1	8:30am – 10:25am Paper Session 4 (4A, 4B, 4C)	8:30am – 10:00am Paper Session 7 (7A, 7B) & Industry Workshop I
	9:30am – 10:00am Break	10:25am – 11:00am Break	10:00am – 10:30am Break
	10:30am – 11:55am Paper Session 1 (1A, 1B, 1C)	11:00am – Noon Keynote Talk 2	10:30am – 11:30am Keynote Talk 3
8:30am – 6:30pm 5 Workshops (W1-W5) & 6 Tutorials (T1-T6) With Coffee Breaks and Lunch	Noon – 1:30pm Lunch on Your Own	Noon – 1:30pm Lunch & Panel: Women in Bioinformatics	11:30am – 1:30pm Lunch & PhD Forum & Industry Workshop II
	1:30pm – 3:05pm Paper Session 2 (2A, 2B, 2C)	1:30pm – 3:05pm Paper Session 5 (5A, 5B, 5C)	
	3:05pm – 3:35pm Break	3:05pm – 3:35pm Break	1:30pm – 5:30pm Health Informatics Symposium & Workshop W6
	3:35pm – 4:40pm Paper Session 3 (3A, 3B, 3C)	3:35pm – 4:25pm Paper Session 6 (6A, 6B, 6C)	
	4:45pm – 5:45pm ACM SIG-BIO Community Meeting	4:30pm – 5:30pm Funding Agency Roundtable	
	6:00pm – 8:30pm Reception/Poster/ Demo/Exhibit	6:00pm – 8:00pm Banquet & Best Paper/Poster Awards	

Sunday, September 22, 2013

Workshops

Workshop W1

8:30am – 6:30pm

Location: Ballroom A

Fourth Immunoinformatics and Computational Immunology Workshop (ICIW 2013)

Vladimir Brusic, Dana-Farber Cancer Institute; Lou Chitkushev, Boston University; Vasant Honavar, Iowa State University; Guanglan Zhang, Boston University; Yasser El-Manzalawy, Iowa State University

8:30am – 9:30am Invited keynote talk by Dr. Bjoern Peters

Discovery of novel T cell antigens in grass pollen through a combined transcriptomic-, proteomic- and immunomic analysis

9:30am – 10:30am Session I (Paper Presentations)

- *iAtheroSim: atherosclerosis process simulator on smart devices.* Francesco Pappalardo, Marzio Pennisi, Ferdinando Chiacchio, Salvatore Musumeci, and Santo Motta.
- *Biomarkers in immunology: from concepts to applications.* Ping Zhang, Lou Chitkushev, Vladimir Brusic, and Guang Lan Zhang.
- *Characterizing Amino Acid Variations in Aligned Pattern Clusters of Scavenger Receptors.* En-Shiun Annie Lee, Fiona Whelan, Dawn Bowdish, and Andrew K. C. Wong.

10:30am – 11:00am Morning break

11:00am – 12:30pm Session II (Paper & Poster Presentations)

- *Landscape of neutralizing assessment of monoclonal antibodies against dengue virus.* Jing Sun, Guang Lan Zhang, Lars Ronn Olsen, Ellis L. Reinherz, and Vladimir Brusic.
- *Predicting protein transport mechanism and immune response using spatial protein motifs and epitopes: a case study of Chlamydomophila MOMP.* F.O. Atanu, E. Oviedo-Orta, and K.A. Watson
- *Enhanced affinity of docking HLA B*57:01 pit with putative self peptide structures by hypersensitivity causative drug of Abacavir and its in silico alikes.* Chen-Chieh Fan, Chun-Fan Chang, Hsueh-Ting Chu, Thai-Yen Ling, and Cheng-Yan Kao.
- *The Two-Faced T Cell Epitope: Examining the Host-Microbe Interface with JanusMatrix.* Andres H. Gutierrez, Chris Bailey-Kellogg, Lenny Moise, Frances Terry, Karim Abdel Hady, Qiben Leng, Marcelo B. Sztein, Phyllis Losikoff, Nathan Verberkmoes, William D. Martin, Alan Rothman, and Anne S. De Groot.
- *In Silico prediction of HLA-DP and -DQ epitope content is poorly correlated with clinical immunogenicity of therapeutic proteins.* A.S. De Groot, R. Tassone, L. P. Cousens, F. Terry, R. Martin, M.T. Ardito, and W.D. Martin.

12:30pm – 2:00pm Lunch**2:00pm – 2:45pm Invited keynote talk by Dr. Steven H Kleinstein***The transcriptional response to influenza infection and vaccination***2:45pm – 4:00pm Session III (Poster Presentations)**

- *Allergenic Proteins Are Targets For Mammalian Ige Mediated Immune Response Against Metazoan Parasites.* Nidhi Tyagi, Stephanie Ryan, Edward Farnell, Colin Fitzsimmons, Rick Maizels, David Dunne, Janet Thornton, and Nicholas Furnham.
- *DNA Vaccine Design For Chikungunya Virus Based On The Conserved Epitopes Derived from Structural Protein.* Parvez Singh Slathia.
- *Highly Immunogenic Vaccine for Prevention and Therapy of Malignant Mesothelioma.* A.S. De Groot, P. Bertino, P. Hoffman, M. Carbone, A.G. Siccardi, F. Terry, L.P. Cousens, L. Moise, and W. Martin.
- *Cross-reactive influenza H1N1 T cell epitopes identified by immunoinformatic methods stimulate CD4+ T cell responses.* Anne S. De Groot, Christine Boyle, Matthew Ardito, Frances Terry, Howard Latimer, Ryan Tassone, Mindy Cote, Leonard Moise, and William D. Martin.

4:00pm – 4:30pm Afternoon Break**4:30pm – 6:30pm Session IV (Tutorials)**

- *iVAX: Interactive Vaccine Design Toolkit.* Willam Martin, Sheila Chandran, Jacob Tivin, Rebecca Tivin.
- *Data mining systems for knowledge discovery in viruses and tumor antigens with direct applications in T-cell immunology and vaccinology.* Guanglan Zhang.
- *ISPRI: In silico high throughput pre-clinical determination of monoclonal antibody immunogenicity.* Willam Martin, Sheila Chandran, Jacob Tivin, Rebecca Tivin.

Workshop W2**8:30am – 5:00pm****Location: Harmony****Computational Structural Bioinformatics Workshop (CSBW 2013)**

Jing He, Old Dominion University; Amarda Shehu, George Mason University; Nurit Haspel, University of Massachusetts; Brian Chen, Lehigh University

8:30am – 10:40am Session I (Session Chair: Nurit Haspel; Co-chair: Bahar Akbal-Delibas)

- 8:30-8:55 Arrival, poster setup
- 8:55-9:00 Welcome and opening remarks (Jing He)
- 9:00-10:00 **Keynote by Dr. Ruth Nussinov**

- 10:00-10:20 *Exploring the Structure Space of Wildtype Ras Guided by Experimental Data*. Rudy Clausen and Amarda Shehu
- 10:20-10:40 *Multi-Resolution Rigidity-Based Sampling of Protein Conformational Paths*. Dong Luo and Nurit Haspel.

10:40am – 11:00am Coffee Break

11:00am – 12:40pm Session II (Session chair: Amarda Shehu; Co-chair: Rudy Clausen)

- 11:00-12:00 **Keynote by Dr. Lenore Cowen**
- 12:00-12:20 *Beta-sheet Detection and Representation from Medium Resolution Cryo-EM Density Maps*. Dong Si and Jing He
- 12:20-12:40 *An Evolutionary Conservation and Rigidity Analysis Machine Learning Approach for Detecting Critical Protein Residues*. Filip Jagodzinski, Bahar Akbal-Delibas and Nurit Haspel.

12:40pm – 2:00pm Lunch

2:00pm – 3:20pm Session III (Session Chair: Brian Chen; Session Co-chair: Dong Si)

- 2:00-2:20 *Fast and Accurate Structure-Based Prediction of Resistance to the HIV-1 Integrase Inhibitor Raltegravir*. Majid Masso.
- 2:20-2:40 *A Combined Molecular Dynamics, Rigidity Analysis Approach for Studying Protein Complexes*. Brian Orndorff and Filip Jagodzinski.
- 2:40-3:00 *Improving the Prediction of Kinase Binding Affinity Using Homology Models*. Jeffrey Chyan, Mark Moll and Lydia Kavrakli.
- 3:00-3:20 *Informatics-driven Protein-protein Docking*. Irina Hashmi and Amarda Shehu.

3:20pm – 4:20pm Poster Session and Coffee Break

4:20pm – 5:00pm Session IV (Session Chair: Jing He; Session Co-chair: Irina Hashmi)

- 4:20-4:40 *A Constrained K-shortest Path Algorithm to Rank the Topologies of the Protein Secondary Structure Elements Detected in CryoEM Volume Maps*. Kamal Al Nasr, Lin Chen and Jing He.
- 4:40-5:00 Poster session
- Closing Remarks (Jing He)

Workshop W3

8:30am – 11:00am

Location: Ballroom C

6th International Workshop on Biomolecular Network Analysis (IWBNA 2013)

Young-Rae Cho, Baylor University; Pietro H. Guzzi, University of Catanzaro, Italy

8:30am – 11:00am

- 8:30 - 8:45 Opening Remarks. Pietro Hiram Guzzi, Young-Rae Cho

- 8:45- 9:15 *Identifying Pathway Proteins in Networks*. Kathryn Dempsey and Hesham Ali.
- 9-15 -9:45 *A Neural-network Algorithm for All k Shortest Paths Problem*. Kun Zhao and Abdoul Sylla.
- 9:45 - 10:15 *Revealing Protein Structures by Co-Occurrence Clustering of Aligned Pattern Clusters*. En-Shiun Annie Lee, Sanderz Fung and Andrew K.C. Wong.
- 10:15 -10:45 *Comparative analysis of network algorithms to address modularity with gene expression temporal data*. Suhaib Mohammed.
- 10:45-11:00 Closing Remarks

Workshop W4

2:00pm – 4:00pm

Location: Ballroom C

Parallel and Cloud-based Bioinformatics and Biomedicine (ParBio 2013)

Mario Cannataro, University Magna Graecia of Catanzaro, Italy

2:00pm – 4:00pm

- 14:00 - 14:15 Opening Remarks, Mario Cannataro
- 14:15 - 14:45 *MEGADOCK-GPU: Acceleration of Protein-Protein Docking Calculation on GPUs*. Takehiro Shimoda; Takashi Ishida; Shuji Suzuki; Masahito Ohue; and Yutaka Akiyama. (Presenter: T. Shimoda, Tokyo Institute of Technology, Japan)
- 14:45 - 15:15 *pXAlign: A parallel implementation of XAlign*. Aditi Magikar; and John Springer. (Presenter: J.A. Springer, Purdue University)
- 15:15 - 15:45 Open discussion on emerging topics in high performance and distributed bioinformatics and biomedicine
- 15:45 - 16:00: Closing Remarks, Mario Cannataro

Workshop W5

9:00am – 12:30pm

Location: Ballroom D

Workshop on Epigenomics and Cell Function (ECF 2013)

David M. Gilbert, Florida State University; Tamer Kahveci, University of Florida

9:00am – 10:30am

- 9:00-10:00 **Keynote by Dr. Frank Alber**

- 10:00-10:30 *Relating mammalian replication program to large-scale chromatin folding*. Benjamin Audit, Antoine Baker, Rasha Boulos, Hanna Julienne, Alain Arneodo, Chun-Long Chen, Yves D'Aubenton-Carafa, Arach Goldar, Guillaume Guilbaud and Olivier Hyrien

10:30am – 11:00am Coffee Break

11:00am – 12:30am

- 11:00-11:30 *Chromatin structure fully determines replication timing program in human cells*. Sven Bilke, Yevgeniy Gindin and Paul Meltzer
- 11:30-12:00 *Unsupervised pattern discovery in human chromatin structure through genomic segmentation*. Michael M. Hoffman, Orion J. Buske, Jie Wang, Zhiping Weng, Jeff Bilmes and William Stafford Noble
- 12:00-12:30 *Bayesian Inference of Spatial Organizations of Chromosomes*. Zhaohui Qin, Ming Hu, Jun Liu, Bing Ren, Ke Deng, Siddarth Selvaraj, Jesse Dixon and Jennifer Fang

Tutorials

Tutorial T1

2:00pm – 6:30pm

Location: Ballroom D

From Robot Motion Planning to Modeling Structures and Motions of Biological Molecules

Amarda Shehu, George Mason University;

Nurit Haspel, University of Massachusetts Boston & Juan Cortés, CNRS, France

Abstract: In the last two decades, great progress has been made in molecular modeling through robotics-inspired computational treatments of biological molecules. Deep mechanistic analogies between articulated robots and biomolecules have allowed robotics researchers to bring forth methods originally developed to address the robot motion planning problem to address and elucidate the relationship between macromolecular structure, dynamics, and function in computational structural biology.

Tight coupling of approaches based on robot motion planning with computational physics and statistical mechanics have resulted in powerful methods capable of elucidating protein-ligand binding, order of secondary structure formation in protein folding, kinetic and thermodynamic properties of folding and equilibrium fluctuations in proteins and RNA, loop motions in proteins, small-scale and large-scale motions in multimodal proteins transitioning between different stable structures, and more.

The objective of this tutorial is to introduce the broad community of researchers and students at ACM BCB to robotics-inspired treatments and methodologies for modeling structures and motions in biomolecules. A comprehensive review of the current state of the art, ranging from the probabilistic roadmap approach to tree-based approaches, will be accompanied with specific detailed highlights and software demonstrations of powerful and recent representative robotics-inspired methods for peptides, proteins, and RNA.

Tutorial T2

8:30am – 10:30am

Location: Ballroom B

Protein Function Prediction: Formulation, Methodology, Evaluation, and Challenges

Predrag Radivojac, Indiana University

Abstract: Understanding protein function is one of the keys to understanding life at the molecular level. It is also important in the context of human disease because many conditions arise as a consequence of alterations of protein function. The recent availability of relatively inexpensive sequencing technology has resulted in thousands of complete or partially sequenced genomes with millions of functionally uncharacterized proteins. Such a large volume of data, combined with the lack of high-throughput experimental assays to functionally annotate proteins, attributes to the growing importance of automated function prediction. In this tutorial, I intend to discuss difficulties in experimentally characterizing protein function, motivate and precisely formulate the protein function prediction problem and then present main computational approaches published thus far. Such methods utilize a variety of different data types, such as protein sequence, protein-protein interactions, gene expression, protein structure, etc. Function prediction will be mainly discussed at the level of the entire protein molecule and from different viewpoints (biochemical, biological, phenotypic). Some time will be devoted to discussing metrics for evaluating protein function prediction. Finally, I will introduce the CAFA challenge dedicated to evaluating protein function prediction and briefly discuss the next CAFA challenge whose start is anticipated for the summer of 2013.

Tutorial T3

11:00am – 1:00pm

Location: Ballroom B

Creating Bioinformatic Workflows within the BioExtract Server Leveraging iPlant Resources

Carol Lushbough, University of South Dakota & Rion Dooley, University of Texas

Abstract: In order to handle the vast quantities of biological data generated by high-throughput experimental technologies, The BioExtract Server (bioextract.org) has leveraged iPlant Collaborative (www.iplantcollaborative.org) functionality to help address big data storage and analysis issues in the bioinformatics field. The BioExtract Server is a Web-based, workflow-enabling system that offers researchers a flexible environment for analyzing genomic data. It provides researchers with the ability to save a series of BioExtract Server tasks (e.g. query a data source, save a data extract, and execute an analytic tool) as a workflow and the opportunity for researchers to share their data extracts, analytic tools and workflows with collaborators. The iPlant Collaborative is a community of researchers, educators, and students working to enrich science through the development of cyberinfrastructure - the physical computing resources, collaborative environment, virtual machine resources, and interoperable analysis software and

data services— that are essential components of modern biology. The iPlant Foundation API, developed through the iPlant Collaborative, is a hosted, Software-as-a-Service resource providing access to a collection of High Performance Computing (HPC) and Cloud resources. Leveraging the iPlant Foundation API, the BioExtract Server gives researchers easy access to multiple high performance computers and delivers computation and storage as dynamically allocated resources via the Internet.

Tutorial T4

2:00pm – 4:00pm

Location: Ballroom B

Transcriptome Assembly and Analysis using RNA-Seq

Dongxiao Zhu and Nan Deng, Wayne State University

Abstract: The ever increasing accumulation of RNA-seq data demands easy-to-use, reliable and scalable analysis software. RNA-seq data is frequently available in standard file formats, such as FASTQ, BED, WIG and SAM/BAM. RNA-seq software must be compatible with these formats. There have been major community efforts on algorithm and software development. Three major categories of tools are currently available: (1) Transcriptome assembly tools, ab initio assembler depends on the reference genome and annotation while de novo assembler does not; (2) Transcriptome quantification tools, either using read counts or exon coverage signal; (3) Transcriptome comparison tools. In this tutorial, we will provide a comprehensive review of the existing computational methods and tools in each category. We will also provide sample RNA-seq data analyses using the selected tools from each category.

Tutorial T5

4:30pm – 6:30pm

Location: Ballroom B

Hands-on Experience with the MIMIC II Database: An Open-Access Database for Knowledge Discovery and Reasoning in Critical Care

Mengling Feng and Thomas Brennan, Massachusetts Institute of Technology

Rob Montgomery, Harvard Medical School & Alan Stein, HP Software

Abstract: Since 2003, our group has been building the Multi-parameter Intelligent Monitoring in Intensive Care II (MIMIC II) Database, which now holds data from about 40,000 ICU admissions. MIMIC II contains vital sign time series, lab results, imaging results, records of medication and fluid administration, staff notes, demographic data and more. Multichannel waveform data is

available for a subset of patients. MIMIC II has been freely shared with the research community via PhysioNet (<http://physionet.org/mimic2>), and we currently have 600 users in over 32 countries.

This hands-on tutorial aims to introduce MIMIC II to the ACM-BCB community. MIMIC II is a valuable resource for research in:

1. Computational Epidemiology/ Evidence-based Medicine
2. Knowledge Representation and Visualization
3. Databases and Ontologies
4. Text Mining and Natural Language Processing
5. Machine Learning and Signal Processing Methods for Physiological Data

In this tutorial, we will introduce The Story Behind MIMIC II. We will also share how MIMIC II has allowed our group to develop predictive models with actionable outputs that may potentially lead to measurable improvement in process and/or outcome. The tutorial will end with A Hands-on Tour of MIMIC II, where participants will learn to navigate through the rich data of MIMIC II. Basic data analytic examples are included to facilitate understanding of MIMIC II data schema.

Tutorial T6

4:30pm – 6:30pm

Location: Ballroom C

GPU Programming for Bioinformatics Applications

Soha Hassoun and Ehsan Ullah, Tufts University

Abstract: The use of Graphics Processing Units (GPUs) has recently emerged as a viable and effective option for compute-intensive scientific applications. The idea here is simple. Instead of using GPUs to speed rendering graphics on the screen for gaming applications, a programmer can utilize the GPUs to solve computationally challenging problems. The GPUs can deliver superb performance owing to hundreds of computing cores grouped into multiprocessors, all connected with impressive memory bandwidth. GPU Speedups (in execution time) have been achieved across multiple scientific application domains, including speedups of 130x for iterative image reconstruction for computational tomography, and 16x to 100x speedup for applications in computational fluid dynamics.

Do you have an application that you would like to speed up using GPUs? This tutorial presents the basic architectural features of GPUs, and basic programming constructs for CUDA™, NVIDIA's parallel computing platform and programming model. A working example based on computing elementary pathways in biochemical networks will be presented to illustrate issues related to CPU to GPU data transfers, effective use of the memory hierarchy, and other GPU-specific optimization techniques. The tutorial caters to programmers who have a background in C/C++ and are interested in speeding up a parallelizable scientific application.

Monday, September 23, 2013

Opening Remarks

8:15am – 8:30am

Location: Grand Ballroom

General Chairs: Cathy Wu, University of Delaware & Sridhar Hannenhalli, University of Maryland

Program Chairs: Donna Slonim, Tufts University & Srinivas Aluru, Georgia Institute of Technology

Keynote Talk 1

8:30am – 9:30am

Location: Grand Ballroom

Session Chair: Cathy Wu, University of Delaware & Georgetown University

How Can Computational Structural Biology Help Cancer Research?

Ruth Nussinov, National Cancer Institute, SAIC-Frederick & Tel Aviv University

Abstract: Structural pathways are important. They are essential to the understanding of how oncogenic mutations work and to figuring out alternative parallel pathways in drug resistant mutants. Structural pathways also help to understand the inter-relationship among linked phenomena, as in the case of inflammation and cancer. Cell biology provides a global overview of the behavior of the cell, tissue and the organism under different sets of conditions; the structures of single proteins and their coherent interactions provide insight into the dynamic changes in the proteins, such as those taking place through post-translational modifications, binding events and mutations, and into their interactions. Nonetheless, beyond the challenging construction of structural pathways, there is also a need to obtain a mechanistic insight into single proteins, their modifications, interactions and broadly, their changing landscapes. Why is insight into the dynamic landscape of single proteins important? Perceiving proteins' behavior can help to forecast allosteric transitions, and regulation, and it can help relate oncogenic mutations to their constitutive consequences. The talk will largely focus on structural pathways related to cancer, and oncogenic mutations mapped on these to figure out their mechanisms. These are some of the ways through which computational structural biology can help cancer research.

9:30am – 10:00am Morning Break

Paper Session 1

10:00am – 11:55am

Session 1A: Protein and RNA Structure I

Location: Ballroom A+B
Session Chair: Alber Frank,
University of Southern California

Session 1B: Machine Learning Applications

Location: Ballroom C
Session Chair: Predrag Radivojac,
Indiana University

Session 1C: Alignments

Location: Ballroom D
Session Chair: Mark Clement,
Brigham Young University

1. **L: 10:00-10:25am**

Flexible RNA design under structure and sequence constraints using formal languages. Yu Zhou, Yann Ponty, Stéphane Vialette, Jerome Waldispuhl, Yi Zhang and Alain Denise.

1. **L: 10:00-10:25am**

MarkovBin: An Algorithm to Cluster Metagenomic Reads Using a Mixture Modeling of Hierarchical Distributions. Tin Nguyen and Dongxiao Zhu.

1. **L: 10:00-10:25am**

Masher: Mapping Long(er) Reads with Hash-based Genome Indexing on GPUs. Anas Abu-Doleh, Erik Saule, Kamer Kaya and Umit Catalyurek.

2. **L: 10:25-10:50am**

MRFy: Remote Homology Detection for Beta-Structural Proteins Using Markov Random Fields and Stochastic Search. Noah Daniels, Andrew Gallant, Norman Ramsey and Lenore Cowen.

2. **L: 10:25-10:50am**

Classifying Immunophenotypes with Templates from Flow Cytometry. Ariful Azad, Arif Khan, Bartek Rajwa, Saumyadipta Pyne and Alex Pothén.

2. **L: 10:25-10:50am**

Suffix-Tree Based Error Correction of NGS Reads Using Multiple Manifestations of an Error. Daniel Savel, Thomas Laframboise, Ananth Grama and Mehmet Koyuturk.

3. **L: 10:50-11:15am**

Protein Structure Refinement by Iterative Fragment Exchange. Debswapna Bhattacharya and Jianlin Cheng.

3. **L: 10:50-11:15am**

Improving discrimination of essential genes by modeling local insertion frequencies in transposon mutagenesis data. Michael DeJesus, Thomas Iøerger.

3. **L: 10:50-11:15am**

Genomic Sequence Fragment Identification using Quasi-Alignment. Anurag Nagar and Michael Hahsler.

4. **L: 11:15-11:40am**

Combinatorial clustering of residue position subsets predicts inhibitor affinity across the human kinome. Drew Bryant, Mark Moll, Paul Finn and Lydia Kavraki.

4. **L: 11:15-11:40am**

An Ensemble Model for Mobile Device based Arrhythmia Detection. Kang Li, Suxin Guo, Jing Gao and Aidong Zhang.

4. **L: 11:15-11:40am**

GLProbs: Aligning multiple sequences adaptively. Yongtao Ye, David Cheung, Yadong Wang, SM Yiu, Qing Zhan, Tak-Wah Lam and Hingfung Ting.

5. **S: 11:40-11:55am**

The Forward Stem Matrix: An Efficient Data Structure for Finding Hairpins in RNA Secondary Structures. Richard Beal, Donald Adjeroh, Ahmed Abbasi.

5. **S: 11:40-11:55am**

Stable Feature Selection with Minimal Independent Dominating Sets. Le Shu, Tianyang Ma and Longin Latecki.

5. **S: 11:40-11:55am**

glu-RNA: aliGn highLy strUctured ncRNAs using only sequence similarity. Prapaporn Techa-Angkoon, Yanni Sun.

**Noon – 1:30pm Lunch
(Lunch on Your Own)**

Paper Session 2

1:30pm – 3:05pm

**Session 2A:
Imaging and Visualization**

Location: Ballroom A+B
Session Chair: May Wang,
Georgia Tech & Emory University

**Session 2B:
Big Data, HPC, and Algorithms**

Location: Ballroom C
Session Chair: Tamer Kahveci,
University of Florida

**Session 2C:
Proteins and Proteomics**

Location: Ballroom D
Session Chair: Lenore Martin,
University of Rhode Island

1. L: 1:30-1:55pm

Quantitative Early Detection of Diabetic Foot. Viktor Chekh, Shuang Luan, Mark Burge, Cesar Carranza, Peter Soliz, Elizabeth McGrew and Simon Barriga.

2. L: 1:55-2:20pm

Performance Model Selection for Learning-based Biological Image Analysis on a Cluster. Jie Zhou, Anthony Brunson, John Winans, Kirk Duffin, Nicholas Karonis

3. S: 2:20-2:35pm

Visual Analytics to Optimize Patient-Population Evidence Delivery for Personalized Care. Ketan Mane, Phillips Owen, Charles Schmitt, Kirk Wilhelmsen, Kenneth Gersing, Ricardo Pietrobon and Igor Akushevich.

4. S: 2:35-2:50pm

An Image-Text Approach for Extracting Experimental Evidence of Protein-Protein Interactions in the Biomedical Literature. Luis Lopez, Jingyi Yu, Cecilia Arighi, Manabu Torii, Vijay Shanker, Hongzhan Huang and Cathy Wu.

1. L: 1:30-1:55pm

TCGA Toolbox: an Open Web App Framework for Distributing Big Data Analysis Pipelines for Cancer Genomics. David Robbins, Alexander Grüneberg, Helena Deus, Murat Tanik, Jonas Almeida

2. L: 1:55-2:20pm

MoTeX: A word-based HPC tool for MoTif eXtraction. Solon Pissis, Alexandros Stamatakis and Pavlos Pavlidis.

3. S: 2:20-2:35pm

Cloud4SNP: Distributed Analysis of SNP Microarray Data on the Cloud. Giuseppe Agapito, Mario Cannataro, Pietro Hiram Guzzi, Fabrizio Marozzo, Domenico Talia and Paolo Trunfio.

4. S: 2:35-2:50pm

Read Annotation Pipeline for High-Throughput Sequencing Data. James Holt, Shunping Huang, Leonard McMillan and Wei Wang.

1. L: 1:30-1:55pm

Meta-analysis of Genomic and Proteomic Features to Predict Synthetic Lethality of Yeast and Human Cancer. Min Wu, Xuejuan Li, Fan Zhang, Xiaoli Li, Chee-Keong Kwoh and Jie Zheng.

2. L: 1:55-2:20pm

Classifying Proteins by Amino Acid Variations of Sequential Patterns. En-Shiun Annie Lee and Andrew KC Wong.

3. S: 2:20-2:35pm

A Framework for Identifying Affinity Classes of Inorganic Materials Binding Peptide Sequences. Nan Du, Marc R Knecht, Paras N Prasad, Mark T Swihart, Tiffany Walsh, Aidong Zhang.

4. S: 2:35-2:50pm

Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface. Brian Olson and Amarda Shehu.

5. S: 2:50-3:05pm

Towards Independent Particle Reconstruction from Cryogenic Transmission Electron Microscopy. Lewis Collier, Jean-Yves Herve', Lenore Martin.

5. S: 2:50-3:05pm

Heuristics for the Sorting by Length-Weighted Inversion Problem. Thiago Da Silva Arruda, Ulisses Dias and Zanoni Dias.

5. S: 2:50-3:05pm

Identifying protein complexes in AP-MS data with negative evidence via soft Markov clustering. Yu-Keng Shih and Srinivasan Parthasarathy

3:05pm – 3:35pm Afternoon Break

Paper Session 3

3:35pm – 4:40pm

**Session 3A:
Evolution &
Comparative Genomics
Location: Ballroom A+B**

Session Chair: Yanni Sun,
Michigan State University

1. L: 3:35-4:00pm

Haplotype-based prediction of gene alleles using pedigrees and SNP genotypes. Yuri Pirola, Gianluca Della Vedova, Paola Bonizzoni, Alessandra Stella and Filippo Biscarini.

2. L: 4:00-4:25pm

Greedy Randomized Search Procedure to Sort Genomes using Symmetric, Almost-Symmetric and Unitary Inversions. Ulisses Dias, Christian Baudet and Zanoni Dias.

3. S: 4:25-4:40pm

Transforming Genomes Using MOD Files with Applications. Shunping Huang, Chia-Yu Kao, Leonard McMillan and Wei Wang.

**Session 3B:
Gene Expression**

Location: Ballroom C
Session Chair: Luis Rueda,
University of Windsor

1. L: 3:35-4:00pm

Optimal timepoint sampling in high-throughput gene expression experiments. Bruce Rosa, Ji Zhang, Ian Major, Wensheng Qin and Jin Chen.

2. L: 4:00-4:25pm

SpliceGrapherXT: From Splice Graphs to Transcripts Using RNA-Seq. Mark Rogers, Christina Boucher and Asa Ben-Hur.

3. S: 4:25-4:40pm

An Island-Based Approach for Differential Expression Analysis. Abdallah Eteleeb, Robert Flight, Benjamin Harrison, Jeffrey Petruska and Eric Rouchka.

**Session 3C:
Network Reconstruction**

Location: Ballroom D
Session Chair: Andy Perkins,
Mississippi State University

1. L: 3:35-4:00pm

Reconstructing transcriptional regulatory networks by probabilistic network component analysis. Jinghua Gu, Jianhua Xuan, Xiao Wang, Ayesha N Shajahan, Leena Hilakivi-Clarke and Robert Clarke.

2. L: 4:00-4:25pm

Large scale signaling network reconstruction. Seyedsasan Hashemikhabir, Eyup Serdar Ayaz, Yusuf Kavurucu, Tolga Can and Tamer Kahveci.

3. S: 4:25-4:40pm

Gene Set Cultural Algorithm: A Cultural Algorithm Approach to Reconstruct Networks from Gene Sets. Thair Judeh, Thair Jayyousi, Lipi Acharya, Robert Reynolds and Dongxiao Zhu.

ACM SIG-BIO Community Meeting

4:45pm-5:45pm

Location: Ballroom D

Session Chair: Aidong Zhang, State University of New York at Buffalo

Reception/Poster/ Demo/Exhibit

6:00pm-8:30pm

Location: Harmony/Balance/Wisdom

List of accepted posters are at the end of this brochure

Tuesday, September 24, 2013

Paper Session 4

8:30am – 10:25am

**Session 4A:
Networks and
Sequence Analysis**
Location: Ballroom A+B
Session Chair: Alex Pothen,
Purdue University

**Session 4B:
Regulation and
Metagenomics**
Location: Ballroom C
Session Chair: T. M. Murali,
Virginia Tech

**Session 4C:
Biomedical Informatics
and Text Mining**
Location: Ballroom D
Session Chair: Yogesh Simmhan,
University of Southern California

1. **L: 8:30-8:55am**

Color distribution can accelerate network alignment. Md Mahmudul Hasan and Tamer Kahveci.

1. **L: 8:30-8:55am**

DiffSplice: the Genome-Wide Detection of Differential Splicing Events with RNA-seq. Yin Hu, Jan Prins and Jinze Liu.

1. **L: 8:30-8:55am**

An Ensemble Topic Model for Sharing Healthcare Data and Predicting Disease Risk. Andrew Rider and Nitesh Chawla.

2. **L: 8:55-9:20am**

Decomposing Biochemical Networks Into Elementary Flux Modes Using Graph Traversal. Soha Hassoun, Ehsan Ullah, Shuchin Aeron and Calvin Hopkins.

2. **L: 8:55-9:20am**

Detecting various types of differential splicing events using RNA-Seq data. Nan Deng and Dongxiao Zhu.

2. **L: 8:55-9:20am**

Temporal Relation Identification and Classification in Clinical Notes. Jennifer D'Souza and Vincent Ng

3. **L: 9:20-9:45am**

PRASE: PageRank-based Active Subnetwork Extraction. Ayat Hatem, Kamer Kaya and Umit Catalyurek.

3. **L: 9:20-9:45am**

Identification of gene clusters with phenotype-dependent expression with application to normal and premature ageing. Kun Wang, Avinash Das, Zheng-Mei Xiong, Kan Cao, Sridhar Hannenhalli.

3. **L: 9:20-9:45am**

Text Mining of Protein Phosphorylation Information Using a Generalizable Rule-Based Approach. Manabu Torii, Cecilia Arighi, Qinghua Wang, Cathy Wu and K Vijay-Shanker.

4. **L: 9:45-10:10am**

SPARCS: a method to analyze (un)structured regions in coding RNA sequences. Yang Zhang, Yann Ponty, Mathieu Blanchette, Eric Lécuyer and Jerome Waldispuhl.

4. **L: 9:45-10:10am**

Spatial Genome Conformation and Gene-Gene Interaction Networks of Human Cells. Zheng Wang, Renzhi Cao, Kristen Taylor, Aaron Briley, Charles Caldwell and Cheng Jianlin.

4. **L: 9:45-10:10am**

The TREC Medical Records Track. Ellen M Vorhees.

5. S: 10:10-10:25am

Fine-Scale Recombination Mapping of High-Throughput Sequence Data.

Catherine Welsh, Chen-Ping Fu, Fernando Pardo-Manuel de Villena and Leonard McMillan.

5. S: 10:10-10:25am

Systematic Assessment of RNA-Seq Quantification Tools Using Simulated Sequence Data. Raghu Chandramohan, Po-Yen Wu, John H Phan and May D Wang.

5. S: 10:10-10:25am

A Privacy Preserving Markov Model for Sequence Classification. Suxin Guo, Sheng Zhong and Aidong Zhang.

10:25am – 11:00am Morning Break**Keynote Talk 2****11:00am – noon****Location: Grand Ballroom**

Session Chair: Donna Slonim, Tufts University

Precision Medicine by Finding the True Names of Disease**Isaac Kohane, Harvard Medical School**

Abstract: A recent IOM report on Precision Medicine articulated the case for using multiple dimensions of measurement, from the molecular to the environmental, all keyed to the individual, to redefine medical taxonomies that are more meaningful for prognosis and therapeutic decision-making. Such an "Information Commons" is an essential step to discovering the true names of the diseases that afflict us and I will first address recent developments that make the Information Commons attainable at a national scale. I will then address several important methodological and cultural obstacles have to be overcome. Beyond the restrictive focus of organ, molecular or phenomenology-based approaches, there are also obstacles created by several methodological disciplines (genomics, bioinformatics, epidemiology, biostatistics) that each claim to take an objective perspective. I will highlight these obstacles through a case history of the definition of the diseases of the autism spectrum disorders. In doing so, I highlight the opportunity and obligations for translational bioinformatics researchers.

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

Panel: Women in Bioinformatics

12:15 – 1:15pm

Location: Ballroom D

Session Chair: May Wang, Georgia Tech & Emory University

Panelists: **Clare Bates Congdon**, University of Southern Maine; **Adriana Compagnoni**, Stevens Institute of Technology; **Debra S Goldberg**, University of Colorado Boulder; **Vanja Paunić**, University of Minnesota; **Louisa Raschid**, University of Maryland; **Ellen M. Voorhees**, National Institute of Standards and Technology; **Catie Welsh**, UNC-Chapel Hill; **Wei Wang**, U California Los Angeles

What is your opinion on growing areas of research in bioinformatics?

What are some challenges woman are facing in bioinformatics?

What are the pros and cons of working in academia?

What are the pros and cons of working in industry?

Are there different skill set required for industry and academic positions?

What are the essential skills students should acquire if they want to pursue research in bioinformatics?

What are the strengths and weaknesses of the current bioinformatics courses and how can they be improved?

What do you think about open vs. closed source research? Additionally, open vs. closed validation and data sharing?

How can we convince more women to enter bioinformatics?

How often you take a post-doc whose graduate work was not in bioinformatics?

What are particular skills do you look for?

Paper Session 5

1:30pm – 3:05pm

**Session 5A:
Biomedical Informatics II**

Location: Ballroom A+B

Session Chair: David Koes,
University of Pittsburgh

**Session 5B:
Alignment and Assembly**

Location: Ballroom C

Session Chair: Kodira Chinnappa,
GE Global Research

**Session 5C:
Protein and RNA Structure II**

Location: Ballroom D

Session Chair: Lenore Cowen, Tufts
University

1. L: 1:30-1:55pm

Binary Response Models for Recognition of Antimicrobial Peptides. Elena Randou, Daniel Veltri and Amarda Shehu.

1. L: 1:30-1:55pm

YOABS: Yet Other Aligner of Biological Sequences - the first $O(n)$ alternative to Smith-Waterman alignment of gapped sequences. Vitaly Galinsky.

1. L: 1:30-1:55pm

Simultaneous determination of subunit and complex structures of symmetric homo-oligomers from ambiguous NMR data. Himanshu Chandola, Bruce Donald and Chris Bailey-Kellogg.

2. L: 1:55-2:20pm

Evaluation of Label Dependency for the Prediction of HLA Genes. Vanja Paunic, Michael Steinbach, Abeer Madbouly and Vipin Kumar.

2. L: 1:55-2:20pm

PERGA: A Paired-End Read Guided De Novo Assembler for Extending Contigs Using SVM Approach. Xiao Zhu, Henry Leung, Francis Chin, SM Yiu, Guangri Quan, Bo Liu and Yadong Wang.

2. L: 1:55-2:20pm

Improving phosphopeptide identification in shotgun proteomics by supervised filtering of peptide-spectrum matches. Sujun Li, Randy Arnold, Haixu Tang and Predrag Radivojac.

3. S: 2:20-2:35pm

Simulating Anti-adhesive and Antibacterial Bifunctional Polymers for Surface Coating using BioScape. Vishakha Sharma, Adriana Compagnoni, Matthew Libera, Agnieszka K Muszanska, Henk JBusscher and Henny C van der Mei.

3. S: 2:20-2:35pm

Application of a MAX-CUT Heuristic to the Contig Orientation Problem in Genome Assembly. Paul Bodily, Mark Clement, Jared Price, Nozomu Okuda, Stanley Fujimoto, Quinn Snell and Cole Lyman.

3. S: 2:20-2:35pm

ChainKnot: a comparative H-type pseudoknot prediction tool using multiple ab initio folding tool. Jikai Lei, Prapaporn Techa-Angkoon, Yanni Sun and Rujira Achawanantakun.

4. S: 2:35-2:50pm

Classification of Alzheimer Diagnosis from ADNI Plasma Biomarker Data. Jue Mo, Stuart Maudsley, Bronwen Martin, Sana Siddiqui, Huey Cheung, Calvin Johnson.

4. S: 2:35-2:50pm

Designing Autocorrelated Genes. Rukhsana Yeasmin, Jesmin Jahan Tithi, Jeffrey Chen and Steven Skiena.

4. S: 2:35-2:50pm

A Confidence Measure for Model Fitting with X-Ray Crystallography Data. Ramgopal Mettu and Yang Lei.

5. S: 2:50-3:05pm

Predictive model of the treatment effect for patients with major depressive disorder. Igor Akushevich, Julia Kravchenko, Ken Gersing and Ketan Mane.

5. S: 2:50-3:05pm

GapsMis: flexible sequence alignment with a bounded number of gaps. Carl Barton, Tomas Flouri, Costas Iliopoulos and Solon Pissis.

5. S: 2:50-3:05pm

GPU-Optimized Hybrid Neighbor/Cell List Algorithm for Coarse-Grained MD Simulations of Protein and RNA Folding and Assembly. Andrew Proctor, Cody Stevens and Samuel Cho.

3:05pm – 3:35pm Afternoon Break

Paper Session 6

3:35pm – 4:25pm

**Session 6A:
Genome Organization and
Variant Detection**

Location: Ballroom A+B

Session Chair: Michael Hoffman,
University of Washington

**Session 6B:
Text Mining and Ontologies**

Location: Ballroom C

Session Chair: Mario Cannataro,
University of Catanzaro

**Session 6C:
Signaling and Metabolic
Networks**

Location: Ballroom D

Session Chair: Chris Bailey-Kellog,
Dartmouth College

1. **L: 3:35-4:00pm**

Topological properties of chromosome conformation graphs reflect spatial proximities within chromatin. Hao Wang, Geet Duggal, Rob Patro, Michelle Girvan, Sridhar Hannenhalli and Carl Kingsford.

1. **L: 3:35-4:00pm**

Measuring Relatedness Between Scientific Entities in Annotation Datasets. Guillermo Palma, Maria-Esther Vidal, Eric Haag, Louiqa Raschid and Andreas Thor.

1. **L: 3:35-4:00pm**

PReach: Reachability in Probabilistic Signaling Networks. Haitham Gabr, Andrei Todor, Helia Zandi, Alin Dobra and Tamer Kahveci.

2. **L: 4:00-4:25pm**

A generalized sparse regression model with adjustment of pedigree structure for variant detection from next generation sequencing data. Shaolong Cao, Huaizhen Qin, Yu-Ping Wang and Hong-Wen Deng.

2. **L: 4:00-4:25pm**

Construction of Protein Phosphorylation Networks by Data Mining, Text Mining, and Ontology Integration: Analysis of the Spindle Checkpoint. Karen Ross, Cecilia Arighi, Jia Ren, Hongzhan Huang, Darren Natale and Cathy Wu.

2. **L: 4:00-4:25pm**

PathCase-MAW: An Online Metabolic Network Analysis Workbench. Ercument Cicek, Xinjian Qi, Ali Cakmak, Stephan R Johnson, Xu Han, Sami Alshalwi and Gultekin Ozsoyoglu.

Funding Agency Roundtable

4:30pm – 5:30pm

Location: Ballroom D

Moderator: Iosif Vaisman, George Mason University

With representatives from NIH, NSF, DOE, USDA, and AFOSR, this panel will present and discuss major initiatives and funding opportunities relating to support for research and education in Bioinformatics, Computational Biology and Biomedical Informatics; covering opportunities for early-career investigators, inter-agency initiatives, and topics such as big data.

Panelists

- Susan K. Gregurick, Director, Division of Biomedical Technology, Bioinformatics, and Computational Biology National Institute of General Medical Sciences (NIGMS), National Institutes of Health (NIH)

- Vasant Honavar, Program Director, Division of Information and Intelligent Systems
Directorate for Computer & Information Science & Engineering (CISE), National Science Foundation (NSF)
- Lakshmi Kumar Matukumalli, National Program Leader, Animal Breeding, Genetics and Genomics
National Institute of Food and Agriculture (NIFA), U.S. Department of Agriculture (USDA)
- Pablo Rabinowicz, Program Manager
Office of Biological & Environmental Research (OBER), Department of Energy (DOE)
- Peter Revesz, Program Manager, Air Force Office of Scientific Research (AFOSR)

Banquet & Best Paper/Poster Awards

6:00pm – 8:00pm

Location: Grand Ballroom

Chair: Sridhar Hannenhalli, University of Maryland

Wednesday, September 25, 2013

Paper Session 7

8:30am – 10:00am

Session 7A: Systems Biology

Location: Ballroom A+B

Session Chair: Yoo-Ah Kim,
NCBI, National Library Medicine

Session 7B: Health Informatics

Location: Ballroom D

Session Chair: Umit Catalyurek,
Ohio State University

1. **L: 8:30-8:55am**

Maximizing the Information Content of Experiments in Systems Biology. Juliane Liepe, Sarah Filippi, Michal Komorowski and Michael Ph Stumpf.

2. **L: 8:55-9:20am**

Global Network Alignment In The Context of Aging. Tijana Milenkovic, Han Zhao and Fazle Faisal.

3. **L: 9:20-9:45am**

Top-Down Network Analysis to Drive Bottom-Up Modeling of Physiological Processes. Christopher Poirel, Richard Rodrigues, Katherine Chen, John Tyson and TM Murali.

4. **S: 9:45-10:00am**

Clustering Coefficients in Protein Interaction Hypernetworks. Suzanne Gallagher and Debra Goldberg.

1. **L: 8:30-8:55am**

Algorithms and Systems for Interactive Online Drug Discovery. David Koes and Carlos Camacho.

2. **L: 8:55-9:20am**

A Semi-Supervised Learning Approach to Integrated Salient Risk Features for Bone Diseases. Hui Li, Xiaoyi Li, Murali Ramanathan and Aidong Zhang.

3. **L: 9:20-9:45am**

A Study of Temporal Action Sequencing During Consumption of a Meal. Raul Ramos-Garcia and Adam Hoover.

Industry Workshop

8:30am – 10:00am & Noon – 1:30pm

Location: Ballroom C

Exploring Big Data in Pharma and Healthcare: Top down or Bottom up?

Session Chairs: Anastasia Christianson, AstraZeneca Pharmaceutical & Michael Liebman, Strategic Medicine

Abstract: Big Data is a common catch-phrase used these days to describe the growing volume of structured and unstructured data in all areas: scientific, business, and everyday-life. We are faced with so much data daily that it exceeds our ability to process and derive knowledge from them using traditional approaches involving database, and software techniques.

Like many of the technological developments over the past 20 years, pharma and the medical communities hold high hopes that big data will help us better understand mechanisms of disease and lead to better therapies. But given the pace that any technological advances have actually yielded high impact, it is time to investigate the interface between biology and information technology and apply a top-down approach to big data exploitation to complement the bottom-up approaches that we have traditionally followed when applying technology to any discipline.

In this workshop, we will discuss examples of how Pharmaceutical, Biotech, and related healthcare industries are making use of big data and we will explore both the top down and bottom up approaches. A series of presentations will be followed by a panel discussion to discuss the opportunities and challenges of big data from an industry perspective as well as potential opportunities in collaborating across domains, industry, academia.

8:30 – 10:00am Industry Workshop Part I

8:30am Chairperson's remarks

8:35 – 10:00am Session I

- 8:35 – 9:00 *Building the context on the relevance/importance of Big Data in Pharma and Healthcare.* Anastasia Christianson, Senior Director, R&D Information, AstraZeneca Pharmaceutical
- 9:00 – 9:25 *Using clinical lab data to inform trial design.* Dimitris Agrafiotis, Vice President, Informatics and Enterprise Architecture, Covance.
- 9:25 – 9:50 *Integration of biological knowledge with molecular and pharmacological data in systematic drug repositioning.* Vinod Kumar, Senior Scientific Investigator, GlaxoSmithKline Pharmaceuticals.

10:00am – 10:30am Morning Break

Keynote Talk 3

10:30am – 11:30am

Location: Grand Ballroom

Session Chair: Srinivas Aluru, Georgia Institute of Technology

Computational Challenges of Next-Generation Genome Sequence Analysis

Steven L. Salzberg, Johns Hopkins University School of Medicine

Abstract: Next-generation sequencing (NGS) technology allows us to peer inside the cell in exquisite detail, revealing new insights into biology, evolution, and disease that would have been impossible to find just a few years ago. The enormous volumes of data

produced by NGS experiments present many computational challenges that we are working to address. In this talk, I will discuss some of the latest solutions to two basic alignment problems: (1) mapping sequences onto the human genome at very high speed, and (2) mapping and assembling transcripts from RNA-seq experiments. I will also discuss some of the problems that can arise during alignment and how these can lead to mistaken conclusions about genetic variation and gene expression.

My group has developed algorithms to solve each of these problems, including the widely-used Bowtie and Bowtie2 programs for fast alignment and the TopHat and Cufflinks programs for assembly and quantification of genes in transcriptome sequencing (RNA-seq) experiments. This talk describes joint work with current and former lab members including Ben Langmead, Cole Trapnell, Daehwan Kim, and Geo Pertea; and with collaborators including Mihai Pop and Lior Pachter.

11:30am – 1:30pm Lunch
(Lunch provided by the conference)

PhD Forum

Noon – 1:30pm

Location: Harmony

Session Chair: Yanni Sun, Michigan State University

The Ph.D. Forum provides an opportunity for students to present and discuss their research both with peers and with a panel of experienced researchers from academia and industry. All students who attend ACM-BCB are encouraged to present posters on their research in this event. In addition to providing feedback and advice, this forum provides a friendly and supportive environment for students to network, practice poster defending skills and exchange ideas on research topics.

Industry Workshop

8:30am – 10:00am & Noon – 1:30pm

Location: Ballroom C

Exploring Big Data in Pharma and Healthcare: Top down or Bottom up?

Session Chairs: Anastasia Christianson, AstraZeneca Pharmaceutical & Michael Liebman, Strategic Medicine

12:00 – 1:30pm Industry Workshop Part II (Bring your conference provided boxed lunch to the session)

12:00pm Chairperson's remarks

12:05 – 12:55pm Session II

- 12:05 – 12:30 *Comparative Effectiveness in Global Medicine: It's Bigger than You Think...* Michael Liebman, Managing Partner, Strategic Medicine
- 12:30 – 12:55 *Big Data in Biosurveillance*. Peter A. Schad, Chief Scientific Officer, Digital Infuzion, Inc.

12:55 – 1:30pm Panel Discussion

Panelists: all speakers (Anastasia Christianson; Michael Liebman; Dimitris Agrafiotis; Vinod Kumar; Peter Schad) and Daniel Ingber, Lead, Clinical & Translational Informatics - R&D IS, MedImmune

During the Panel discussion, we will elaborate on the challenges and opportunities of big data in industry. The following are possible questions we could tackle in the panel discussion plus, of course, questions from the audience.

- When we say big data what do we really mean in the context of our work? What type of big data are we using?
- What about top down versus bottom up approaches – which ones are you using and why?
- What are the greatest challenges of using big data?
- How can we overcome challenges?
- What are the greatest benefits so far; anticipated and real/already achieved?
- What do you think is the promise of big data in 5-10 years?

Workshop W6

1:30pm – 5:30pm

Location: Ballroom D

Challenges in Accelerating Next-Gen Sequencing Bioinformatics (NGS 2013)

Session Chairs: Shel Swenson & Viktor Prasanna, University of Southern California

Abstract: There is a vital need and present opportunity to develop a community-based collaborative software infrastructure that aims to accelerate the design, implementation, optimization, and dissemination of a wide variety of NGS-enabled codes tuned for accelerator-based systems, as well as methodologies, education and training materials. The goal of this workshop is to explore these research challenges, both from a computer science as well as an applications perspective, and to develop a community research agenda, including identifying requirements and best practices, establishing community cases and bench marks, identifying software frameworks tools, and creating community forums for exchange of ideas and artifacts. This workshop is part a broader NSF Sustainable Software Innovation Institute Conceptualization project entitled "Software Infrastructure for Accelerating Grand Challenge Science with Future Computing Platforms" future-compute.usc.edu, supported by NSF BIO and CISE directorates.

1:30 – 2:15pm Opening Remarks and Introduction

- *Leveraging future computing platforms to accelerate data-intensive grand challenge Problems*. Speakers include Viktor Prasanna, Yogesh Simmhan, and Inanc Birol

2:15 – 2:30pm Coffee Break

2:30– 3:45pm Breakout Session I

- 2:30 – 3:30 *Exploring specific NGS-enabled applications with opportunities for graph abstractions and future computing platforms* (Facilitator: Shel Swenson)
- 3:30 – 3:45 Breakout Session I Report

3:45 – 4:00pm Coffee Break

4:00 – 5:15pm Breakout Session II

- 4:00 – 5:00 *Challenges and solutions in developing sustainable accelerated NGS bioinformatics applications* (Facilitator: Yogesh Simmhan)
- 5:00 – 5:15 Breakout Session II Report

5:15 – 5:30pm Outline Report and Concluding Remarks (Shel Swenson and Viktor Prasanna)

Health Informatics Symposium

1:30pm – 5:30pm

Location: Ballroom A+B

Session Chairs: Maricel Kann, University of Maryland Baltimore County & Philip Payne, Ohio State University

1:30 – 2:30pm Clinical and Translational Research

- 1:30 – 2:00 *Aggregating Personal Health Messages for Scalable Comparative Effectiveness Research*. Jason H.D. Cho, Vera Q.Z. Liao, Yunliang Jiang and Bruce Schatz.
- 2:00 – 2:30 *Evidence of a Pathway of Reduction in Bacteria: Reduced Quantities of Restriction Sites Impact tRNA Activity in a Trial Set*. Oliver Bonham-Carter, Lotfollah Najjar and Dhundy Bastola.

2:30 – 2:45pm Coffee Break

2:45– 3:45pm Information Extraction

- 2:45 – 3:15 *Locating Discharge Medications in Natural Language Summaries*. Simon Diemert, Morgan Price and Jens Weber.
- 3:15 – 3:45 *Modeling Incidental Findings in Radiology Records*. Eamon Johnson, W Christopher Baughman and Gultekin Ozsoyoglu.

3:45 – 4:00pm Coffee Break

4:00– 5:30pm Clinical Informatics

- 4:00 – 4:30 *Mobility Patterns of Doctors Using Electronic Health Records on iPads*. Allan Lin, Mike Chen, Meng-Hsiu Chang, Travis Yu, Lih-Ching Chou, Dian-Je Tsai and Jackey Wang.
- 4:30 – 5:00 *Enforcing Minimum Necessary Access in Healthcare through Integrated Audit and Access Control*. Paul Martin, Avi Rubin and Rafae Bhatti.
- 5:00 – 5:30 *GaitTrack: Health Monitoring of Body Motion from Spatio-Temporal Parameters of Simple Smart Phones*. Joshua Juen, Qian Cheng, Yanen Li, Valentin Prieto-Centurion, Jerry Krishnan and Bruce Schatz.

Posters

1. *Molecular modeling and docking of some coumarin derivatives as β -secretase inhibitors.* Mohsen Yazdani, Abolfazl Barzegar and Mohammad Ali Hosseinpour Faizi.
2. *Predicting protein transport mechanism and immune response using spatial protein motifs and epitopes: a case study of *Chlamydomophila* MOMP.* Francis O Atanu, Ernesto Oviedo-Orta and Kimberly A Watson.
3. *In silico Analysis of Autoimmune Diseases and Genetic Relationships to Vaccination against Infectious Diseases.* Peter McGarvey, Baris Suzek, James Baraniuk, Shruti Rao, Samir Lababidi, Andrea Sutherland, Richard Forshee and Subha Madhavan.
4. *Modularity and community detection in Semantic Similarity Networks through Spectral Based Transformation and Markov Clustering.* Pietro Hiram Guzzi, Pierangelo Veltri and Mario Cannataro.
5. *Age-Specific Signatures of Glioblastoma at the Genomic, Genetic, and Epigenetic Levels.* Serdar Bozdogan, Aiguo Li, Gregory Riddick, Yuri Kotliarov, Mehmet Baysan, Fabio Iwamoto, Margaret Cam, Svetlana Kotliarova and Howard Fine.
6. *SNP2Structure: A public database for mapping and modeling nsSNPs on human protein structures.* Difei Wang, Kevin Rosso, Shruti Rao, Shailendra Singh, Lei Song, Michael Harris, Varun Singh and Subha Madhavan.
7. *An integrated pharmacogenomic analysis of gemcitabine response using genotype information on DMET genes.* Krithika Bhuvaneshwar, Michael Harris, Thanmozhi Natarajan, Laura Sheahan, Difei Wang, Mahlet Tadesse, Subha Madhavan and John Deeken.
8. *BALMNet: Biologically Associated Text Miner and Network builder.* Ilya Zhbannikov, James Foster, Samuel Hunter, Helena Mendes-Soares, Roxana Hickey and Matthew Settles.
9. *Classifying Proteins by Amino Acid Variations of Sequence Patterns.* En-Shiun Annie Lee.
10. *Global network alignment in the context of aging.* Tijana Milenkovic, Han Zhao and Fazle Faisal.
11. *Dynamic networks reveal key players in aging.* Fazle Faisal and Tijana Milenkovic.
12. *Computational methods for alternative splicing detection using RNA-seq.* Ruolin Liu and Julie Dickerson.
13. *Computer Assisted Surgery-Planning for Microwave Ablation.* Xi Wen, Hong Wang and Weiming Zhai.
14. *GASP: A Greedy Alanine Scanning Peptide design algorithm.* Daniel Zaidman and Haim Wolfson.
15. *Improvement of protein-protein interaction prediction by integrating template-based and template-free protein docking.* Masahito Ohue, Yuri Matsuzaki, Takehiro Shimoda, Takashi Ishida and Yutaka Akiyama.
16. *The MEGADOCK project: Ultra-high-performance protein-protein interaction prediction tools on supercomputing environments.* Takehiro Shimoda, Masahito Ohue, Yuri Matsuzaki, Takayuki Fujiwara, Nobuyuki Uchikoga, Takashi Ishida and Yutaka Akiyama.
17. *Semi-automated Constraint-based Metabolic Model Generation.* Jesse Walsh and Julie Dickerson.
18. *Incorporating Gene Annotations as Node Metadata to Improve Network Centrality Measures for Better Node Ranking.* Divya Mistry and Julie Dickerson.
19. *Using SVM to Predict CCS Read Accuracy and Improve Quality Control for PacBio RS.* Xiaoli Jiao.
20. *Methods for Mutation Analysis and Interpretation.* Erin Boggess and Julie Dickerson.
21. *Protein-protein Docking Using Information from Native Interaction Sites.* Irina Hashmi and Amarda Shehu.
22. *Determining miRNA-disease associations using Bipartite Graph Modelling.* Joseph Nalluri, Bhanu Kamapantula, Debmalya Barh, Preetam Ghosh, Neha Jain, Lucky Juneja and Neha Barve.
23. *Allergenic Proteins Are Targets for Mammalian IgE Mediated Immune Response Against Metazoan Parasites.* Nidhi Tyagi.
24. *Statistical Methods for Ambiguous Sequence Mappings.* Tamer Aldwairi, Andy Perkins, Bindu Nanduri, Mahalingam Ramkumar, Dilip Gautam and Michael Johnson.

25. *ngPhylo - N-Gram Modeled Proteins with Substitution Matrices for Phylogenetic Analysis*. Brigitte Hofmeister and Brian King.
26. *Automated protein structure refinement using i3Drefine software and its assessment in CASP10*. Debswapna Bhattacharya and Jianlin Cheng.
27. *A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein*. Rudy Clausen and Amarda Shehu.
28. *A Novel Algorithm for Feature Detection and Hiding from Ultrasound Images*. Haris Godil, Sonya Davey and Raj Shekhar.
29. *Pan-genome: the infrastructure for bacterial genomes representation and analysis*. Leonid Zaslavsky, Boris Fedorov and Tatiana Tatusova.
30. *Using Machine Learning to Predict the Health of HIV-Infected Patients*. Charles Cole and Brian King.
31. *Evaluation of bioinformatics tools to identify alternative splicing events using RNA-seq data in skeletal muscle differentiation*. Xianlu Peng, Lu Ji, Jiajian Zhou, Huating Wang and Hao Sun.
32. *Detecting differential splicing events with revealing mechanisms using RNA-Seq*. Nan Deng and Dongxiao Zhu.
33. *SASeq: A Selective and Adaptive Shrinkage Approach to Identify and Quantify Condition-Specific Transcripts using RNA-Seq*. Tin Nguyen, Nan Deng and Dongxiao Zhu.
34. *SPATA: A Seeding and Patching Algorithm for Hybrid Transcriptome Assembly*. Tin Nguyen, Zhiyu Zhao and Dongxiao Zhu.
35. *Initial Results In Using de Novo Motif Inference to Detect Cis-Regulatory Modules*. Jeffrey Thompson and Clare Bates Congdon.
36. *Comparative network analysis of gene co-expression networks reveals the conserved and species-specific functions of cell-wall related genes between Arabidopsis and Poplar*. Daifeng Wang, Eric Pan, Gang Fang, Sunita Kumari, Fei He, Doreen Ware, Sergei Maslov and Mark Gerstein.
37. *Reachability analysis in large probabilistic biological networks*. Haitham Gabr, Andrei Todor, Alin Dobra and Tamer Kahveci.
38. *Scheduling of virtual screening application on multi-user pilot-agent platform on grid/cloud to optimize the stretch*. Quang Bui, Emmanuel Medernach, Vincent Breton, Hong Quang Nguyen and Quoc Long Pham.
39. *Exploring local features and the Bag-of-Visual-Words Method for BiImage Classification*. Afzal Godil.
40. *Quality of Care in Critical Access Hospitals*. Arshia Khan and John Grillo.
41. *Prediction of Biological Protein-protein Interaction Types Using Short-Linear Motifs*. Manish Pandit, Luis Rueda and Alioune Ngom.
42. *Results of an International Inter-laboratory 16S rRNA Gene Microbial Identification Study*. Nate Olson and Jayne Morrow.
43. *Conditional Random Field for Candidate Gene Prioritization*. Bingqing Xie, Gady Agam, Natalia Maltsev and Conrad Gilliam.
44. *Quantum Sequence Analysis: A New Alignment-free Technique for Analyzing Sequences in Feature Space*. Mosaab Daoud.
45. *Predicting Breast Cancer Patient Survival Using Machine Learning*. David Solti and Haijun Zhai.
46. *ngsShoRT: A Software for Pre-processing Illumina Short Read Sequences for De Novo Genome Assembly*. Chuming Chen, Sari Khaleel, Hongzhan Huang and Cathy Wu.
47. *Probabilistic Gene Coordination: A New Approach to Infer Co-regulation between Amino Acid Transporters and Metabolic Enzymes*. Eman Badr, Lenwood Heath and Guillaume Pilot.
48. *Quality of Care and Electronic Health Record Systems*. Arshia Khan and John Grillo.
49. *Sparse and Stable Reconstruction of Genetic Regulatory Networks Using Time Series Gene Expression Data*. Roozbeh Manshaei and Matthew Kyan.
50. *Listing Sorting Sequences of Reversals and Translocations*. Amritanjali and G Sahoo.
51. *An overview on Semantic Analysis of Proteomics Data*. Pietro Hiram Guzzi, Marco Mina, Concettina Guerra and Mario Cannataro.
52. *decisivator: an R infrastructure package that addresses the problem of phylogenetic decisiveness*. Ilya Zhbannikov, Joseph Brown and James Foster.

53. *Estimating the Number of Manually Segmented Cellular Objects Required to Evaluate the Performance of a Segmentation Algorithm*. Adele Peskin, Joe Chalfoun, Karen Kafadar and John Elliott.

54. *The Effects of Non-Inhibitory Serpin Maspin on Cell Migration Using An Artificial Neural Network*. Mohammad Abdullah Al-Mamun, M Alamgir Hossain, Charles Fall and Rosemary Bass.

55. *Abstraction of Kinetic Models for Biochemical Networks*. Calvin Hopkins and Soha Hassoun.

56. *Co-occurrence Clusters of Aligned Pattern Clusters*. Sanderz Fung.

57. *Three-Dimensional Spot Detection in Ratiometric Fluorescence Imaging For Measurement of Subcellular Organelles*. William Lau, Sara Lioi, Calvin Johnson and Joseph Mindell.

58. *Evaluating theoretical models of protein interaction network evolution without seed graphs*. Todd A. Gibson and Debra S. Goldberg.

59. *The Atomizer: Extracting Implicit Molecular Structure from Reaction Network Models*. Jose Juan Tapia and James Faeder.

60. *Studies of biological networks with statistical model checking: application to immune system cells*. Natasa Miskov-Zivanov, Paolo Zuliani, Edmund Clarke and James Faeder.

61. *An Algorithm for Constructing Hypothetical Evolutionary Trees Using Common Mutations Similarity Matrices*. Peter Revesz.

62. *Predicting Protein Families using Protein Shape Context*. Jun Tan and Donald Adjero.

Demos/Exhibits

1. ImmPort - Immunology Database and Analysis Portal
2. KBase: An Integrated Knowledgebase for Predictive Biology
3. Online Tools for Collaborative Cross
4. DAVID Bioinformatics Resources
5. CPTAC Data Portal

Area Chairs

Bioimage Analysis

Robert Murphy

Carnegie Mellon University

Badri Roysam

University of Houston

Biomedical Informatics

Philip Payne

Ohio State University

Joel Saltz

Emory University

Data and Knowledge Bases, Text Mining, and Ontologies

Judith Blake

The Jackson Laboratory

Kevin B. Cohen

University of Colorado

Evolution, Population, and Comparative Genomics

Anne Bergeron

University of Quebec

Dan Gusfield

University of California at Davis

Functional Genomics

Curtis Huttenhower

Harvard School of Public Health

Teresa Przytycka

National Library of Medicine, NIH

Gene Regulation and Transcription

Manuel Garber

University of Massachusetts Medical School

Lior Pachter

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Siddhartha Jonnalagadda, Mayo Clinic

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Maricel Kann, University of Maryland
Baltimore Country

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Ramana Madupu, J. Craig Venter
Institute

Noel Malod-Dognin, Imperial College

Vesna Memisevic, Biotechnology HPC
Software Applications Institute

Ramgopal Mettu, Tulane University

Tijana Milenkovic, University of Notre
Dame

Bernard Moret, EPFL

Luay Nakhleh, Rice University

Darren Natale, Georgetown University

Tim Nattkemper, Bielefeld University

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Uwe Ohler, Duke University

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Jaroslav Zola, Rutgers University

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Message from the General Chairs

It is our pleasure to welcome you to the 2013 ACM Conference on Bioinformatics, Computational Biology and Biomedical Informatics (ACM BCB-2013). ACM BCB is the flagship conference of the ACM SIGBio (Special Interest Group on Bioinformatics, Computational Biology and Biomedical Informatics). Now in its fourth year, ACM BCB has established itself as a premier annual forum for promoting multidisciplinary research and development in Bioinformatics, Computational Biology and Biomedicine from academia, industry and government.

Expecting nearly 280 meeting attendees, ACM BCB-2013 promises to be a great conference with world-renowned scientists as keynote speakers, contributed talks at a highly competitive acceptance rate, and the broad participation of the research community serving on the program committee and the organizing committees for workshops, tutorials, and panels. The program features three highly anticipated keynote lectures by Drs. Kohane, Nussinov, and Salzberg. A total of 43 regular papers and 28 short papers were selected after a rigorous review process from about 150 submissions, covering topics ranging from comparative genomics, protein and RNA structure, to network reconstruction and medical informatics. The program also features 11 contributed highlight papers, 62 posters, 5 demos, 6 tutorials, as well as 7 workshops on special topics such as immunoinformatics, structural bioinformatics, and next-gen sequencing bioinformatics. In addition to Conference Proceedings, special issues of selected papers will be published in the IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB) and the Database journal.

With the merging of the ACM SIGHIT into the SIGBio, this year also marks the new addition of a symposium dedicated to Health Informatics. Another new addition is the Industry Workshop to foster potential collaboration across industry and academia. Three special panels on Funding Agency Roundtable, Women in Bioinformatics and PhD Forum help students and faculty navigate the career and funding maze.

We wish to thank all of the authors who submitted papers and participated in the conference. Our deepest appreciation goes to the 100+ researchers who served on the various committees or helped assess the submitted papers. The conference would not be possible without generous gift of time by many people serving on the organizing committee. The essence of a scientific conference is its technical program. Thanks to Drs. Donna Slonim, Srinivas Aluru, and other area chairs, program committee members and reviewers for a diligent and fair review process. Thanks to Dr. Catalyurek for organizing the workshops, Drs. Honavar and Congdon for the tutorials, Drs. Zhu and Wang for the posters, and Drs. Kann and Payne for putting together the Health Informatics Symposium.

We thank other members of the organizing committee – Drs. Christianson, Liebman, Wang, Vaisman, Sun, Cheng, Ghosh, Gao, and Edwards, for their generous help. Special thanks to Drs. Florea and Shehu for spearheading the local organization, and Kang Li for prompt and excellent management of the website. Last but not the least, we thank the Steering Committee, especially Dr. Aidong Zhang for imparting her institutional memory and wisdom; she was always available to provide feedback and her help was invaluable.

Thanks to the generous funding support from the National Science Foundation, we are able to provide partial financial support to 30 student attendees, many from underrepresented groups. We are also delighted to present the ACM SIGBio Best Paper, Best Student Paper, and Best Poster Awards.

On behalf of the organizing committee, we welcome you to Washington, D.C., and wish you an enjoyable and productive meeting.

Cathy Wu and Sridhar Hannenhalli

General Chairs

ACM BCB-2013

Notes

Notes

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