



The Third International Conference on Mathematical and Computational Medicine

May 16 – 18, 2016

The Blackwell Inn and Conference Center | Columbus, Ohio, United States

Welcome!



When your child needs a hospital, everything matters.™

Keynote Speakers:

Monday, May 16, 2016

Predicting Protein Structures by Melding Vague Directives with Molecular Dynamics



Ken Dill, PhD, studies the physics of protein folding, the statistical mechanics of water, principles of nonequilibrium statistical thermodynamics in small systems, and the mechanisms and evolution of cells. His work contributed to understanding that protein folding occurs on funnel-shaped energy landscapes and that protein structures are largely determined by hydrophobic interactions. With Dr. Ron Zuckermann, he developed *peptoids*, a new class of polymer materials that have protein-like properties. With Sarina Bromberg, he co-authored *Molecular Driving Forces*, a textbook in physical chemistry and statistical mechanics. Dill is a Distinguished Professor of Physics and Chemistry, the Louis and Beatrice Laufer Chair of Physical Biology, and Director of the Laufer

Center for Physical and Quantitative Biology at Stony Brook University. He is a member of the National Academy of Sciences and the American Academy of Arts and Sciences, past-president of the Biophysical Society, and has received the Hans Neurath Award from the Protein Society and the Emily Gray Award from the Biophysical Society.

Wednesday, May 18, 2016

Big Data in Biomedicine – Has Anything Fundamentally Changed?



Philip Bourne, PhD, is the Associate Director for Data Science at the National Institutes of Health in the Office of the Director. Prior to coming to NIH, Dr. Bourne was Associate Vice Chancellor for Innovation and Industry Alliances of the Office of Research Affairs and a Professor in the Department of Pharmacology at the University of California at San Diego. Dr. Bourne is a Past President of the International Society for Computational Biology, an elected fellow of the American Association for the Advancement of Science (AAAS), the International Society for Computational Biology (ISCB) and the American Medical Informatics Association (AMIA).

Plenary Presentations:

Monday, May 16, 2016

Human Population Genetics, Mathematical Models, and Genetic Studies of Disease



Noah Rosenberg, PhD, is Professor in the Department of Biology at Stanford University, where he holds the Stanford Professorship in Population Genetics and Society. Prof. Rosenberg's areas of interest include human evolutionary genetics, mathematical phylogenetics, theoretical population genetics, and the relationship of human evolution to the search for disease genes. He currently serves on editorial boards for the journals *Genetics*, *Human Biology*, and *Evolution, Medicine & Public Health*, and he is the editor-in-chief of *Theoretical Population Biology*. Prof. Rosenberg received his BA in mathematics from Rice University and his MS in mathematics and PhD in biology from Stanford University, and he completed postdoctoral work at the University of Southern California. He previously served on the human genetics faculty of the University of Michigan. Population genetics is the study of genetic variation in

populations, and the history underlying that variation. Recent successes in the discovery of genetic risk variants for diverse human disease phenotypes in many ways reflect principles and methods that trace to mathematical models in population genetics. This talk will discuss a number of aspects of the impact of population genetics in the effort to understand the genetic basis of human disease, highlighting the value of mathematical modeling contributions.

Functional Multiple-set Canonical Correlation Analysis: A Method for Integrating Various Sources of Functional Data



Heungsun Hwang, PhD is Associate Professor of Psychology at McGill University. He earned his PhD in Quantitative Psychology from McGill University. He was previously Assistant Professor of Marketing at HEC Montreal and Research Analyst at an international marketing consulting firm. He currently serves on the editorial boards of *Psychometrika*, *Behaviormetrika*, *IEEK Transactions on Smart Processing and Computing*, and *Frontiers in Quantitative Psychology and Measurement*. His research interests include multivariate and functional data analysis, structural equation modeling, cluster analysis, statistical learning, data integration, and neuroimaging and genetic data analysis.

Tuesday, May 17, 2016

Nanoindentation of Virus Capsids in a Molecular Model



Marek Cieplak, PhD, Head, Laboratory of Biological Physics, Institute of Physics, Polish Academy of Sciences in Warsaw, Poland.

Education - M.S., Department of Physics, University of Warsaw, 1973; Ph. D., Department of Physics, University of Pittsburgh, 1977; D.Sc., Department of Physics, University of Warsaw, 1984. Professorial title, 1994.

Fields of interest – condensed matter theory (spin waves, spin glasses, porous media, growth processes, atomic friction, river networks, nanofluidics, self-organized nanostructures) and biological physics (large conformational changes of biomolecules within coarse-grained models, especially as induced by stretching, proteins with knots and slipknots, protein folding, dynamics of virus capsids and other multi-proteinic structures such as a cellulosome, interaction of proteins with solids, proteins at air-water interface, modeling of proteasomes, inference of genetic networks from the microarray data). Textbook “Theory of Quanta” with I. Białyński-Birula and Jerzy Kamiński (Polish Scientific Company -1991, 2001; Oxford University Press -1992). Co-editor of EPL . On the advisory board of Journal of Physics: Condensed Matter. Fellow of the American Physical Society (1998) and its Outstanding Referee (2008). Summer lectures at Rutgers University 1991-2000 and at Johns Hopkins University, since 2001. Many Polish grants; in several European projects (such as NaPa, Funmol, CellulosomePlus, MissingLink). 245 research papers. Hirsch factor 38.

How to Hit HIV Where It Hurts



Arup K. Chakraborty, PhD is the Robert T. Haslam Professor of Chemical Engineering, Physics, Chemistry, and Biological Engineering at MIT. He is the founding Director of MIT’s Institute for Medical Engineering and Science. He is also a founding steering committee member of the Ragon Institute of MIT, MGH, and Harvard, and an Associate Member of the Broad Institute of MIT & Harvard. After obtaining his PhD in chemical engineering at the University of Delaware, and postdoctoral studies at the University of Minnesota, he joined the faculty at the University of California at Berkeley in December 1988. He rose through the ranks, and ultimately served as the Warren and Katherine Schlinger Distinguished Professor and Chair of Chemical Engineering, Professor of Chemistry, and Professor of Biophysics at Berkeley. He was also Head of Theoretical and Computational Biology at Lawrence Berkeley National Laboratory. In September 2005, Arup moved to MIT.

After a successful early career working on molecular engineering of catalysts and polymers, Arup turned his attention to immunology. The central theme of his research over the past fifteen years is the development and application of theoretical/computational approaches, rooted in physics and engineering, to aid the quest for mechanistic principles in immunology, and then harness this understanding to aid the design of vaccines against mutable pathogens (e.g., HIV). A characteristic of his work is the impact of his studies on experimental immunology and clinical studies (he collaborates extensively with leading immunologists). Arup’s work at the interface of the physical, life, and engineering sciences has been recognized by many honors that include a *NIH Director’s Pioneer Award*, the *E.O. Lawrence Memorial Award for Life Sciences*, the *Allan P. Colburn and Professional Progress awards* of the American Institute of Chemical Engineers, a *Camille Dreyfus Teacher-Scholar award*, a Miller Research Professorship, and a *National Young Investigator award*. Arup is a member of the *National Academy of Engineering* and a Fellow of the *American Academy of Arts & Sciences* and the *American Association for the Advancement of Science*. He is also a member of the US Defense Science Board.

Wednesday, May 18, 2016

Measurement scale and dissipation of information shape biological pattern



Steven A. Frank received his PhD in Biology from the University of Michigan. He was a Miller Research Fellow at the University of California, Berkeley, and then joined the faculty at the University of California, Irvine, where he is currently UCI Distinguished Professor of Biological Sciences. Professor Frank develops mathematical, computational, and conceptual models to study natural selection and the evolution of organismal design. His work makes testable predictions on topics ranging from microbial life history to sociality to cancer. His study of particular topics leads to syntheses of natural selection, robustness in relation to biological design, and the commonly observed patterns that emerge from information flow and scale. Information about Professor Frank's research and publications is available at <http://stevefrank.org>.

Exploring Hollywood's Tools for Biovisualization: Data Exploration, Working Models and Communication



Gaël McGill, PhD

Faculty & Director of Molecular Visualization, Harvard Medical School
Founder & CEO, Digizyme Inc.

Dr. Gaël McGill is faculty and Director of Molecular Visualization at Harvard Medical School where his teaching and research focuses on visualization design methods in science education. He is also founder & CEO of [Digizyme, Inc.](http://Digizyme, Inc) a firm dedicated to the visualization and communication of science. Dr. McGill recently co-authored and served as digital director for E.O. Wilson's Life on Earth iPad biology textbook developed in partnership with Apple. He is the creator of the scientific visualization online community portal Clarafi.com (originally molecularmovies.com), the Molecular Maya (mMaya) software toolkit and has contributed to leading Maya and ZBrush textbooks for Wiley/SYBEX Publishing. Dr. McGill is also a board member of the Vesalius Trust and an advisor to several biotechnology and device companies. After his B.A. summa cum laude in Biology, Music, and Art History from Swarthmore College, and Ph.D. in Cell Biology & Biochemistry at Harvard Medical School as a Howard Hughes Medical Institute, Dr. McGill completed his postdoctoral work at the Dana Farber Cancer Institute studying tumor cell apoptosis and melanoma.

The Third International Conference on Mathematical and Computational Medicine

Monday, May 16, 2016

Day 1

- 8:00 - 8:30 **Registration/Check-in**
- 8:30 - 8:45 **Welcome & Opening Remarks - Veronica Vieland, PhD**
- 8:45 - 9:30 **Keynote Speaker**
Ken Dill, PhD - Stony Brook University
"Computing Protein Structures by Combining Molecular Dynamics with Fuzzy Knowledge"

GENETICS and GENOMICS - Chairs: Stewart & Greenberg

- 9:30 - 10:10 **Noah Rosenberg, PhD - Stanford University**
- 10:10 - 10:35 **Michael Epstein, PhD - Emory University**
"A Statistical Approach for Testing Cross-Phenotype Effects of Rare Variants"
- 10:35 - 10:50 **BREAK**
- 10:50 - 11:15 **Paul Scheet, PhD - MD Anderson**
"Sensitive Profiling of Allelic Imbalance Across Tissues for Insights into Early Disease Pathology"
- 11:15 - 11:40 **Susan E. Hodge, DSc - Nationwide Children's Hospital and The Ohio State University**
"Can Gene-Gene Interactions Explain Very Low Odds Ratios in Association Studies?"
- 11:40 - 12:05 **Shili Lin, PhD - The Ohio State University**
"BCurve: Detection of Differentially Methylated Regions Using BS-seq Data Based on Bayesian Credible Bands"
- 12:05 - 12:30 **Wladek Minor, PhD - University of Virginia**
- 12:30 - 12:55 **Maga Rowicka - University of Texas Medical Branch**
"Inferring DSB Causing Factors from Sequencing Read Patterns"
- 12:55 - 1:05 **Spotlight Poster Presentations**
- 1:05 - 2:40 **LUNCH & FREE TIME - (Optional - "Your First Faculty Appointment")**

BIOMARKERS DISCOVERY, OUTCOMES MEASURE, PHENOTYPES - Chairs: Jeon & Bartlett

- 2:40 - 3:20 **Heungsun Hwang, PhD - McGill University**
- 3:20 - 3:45 **Min-Jeong Jeon, PhD - The Ohio State University**
- 3:45 - 4:10 **Colleen Clancy, PhD - University of California, Davis**
"A Computational Pipeline for Safety Pharmacology: From Chemistry to Rhythm"
- 4:10 - 4:25 **BREAK**
- 4:25 - 4:50 **Kun Huang, PhD - The Ohio State University**
- 4:50 - 5:15 **Gaurav Chopra, PhD - Purdue University**
"Interactome-based Drug Discovery and Disease-Disease Relationships"
- 5:15 - 5:40 **Meng Wang, PhD - Nationwide Children's Hospital**
- 5:40 - 6:05 **Grzegorz Rempala, PhD - The Ohio State University**
- 6:05 - 6:20 **Philip Payne, PhD - The Ohio State University**

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Tuesday, May 17, 2016

Day 2

PROTEINS - Chair: Cieplak

- 8:30 - 9:10 **Marek Cieplak, PhD - Institute of Physics, Polish Academy of Sciences**
- 9:10 - 9:35 **Daisuke Kihara, PhD - Purdue University**
"Ensemble-based Evaluation for Protein Structure Models"
- 9:35 - 10:00 **Jarek Meller, PhD - University of Cincinnati**
- 10:00 - 10:15 **BREAK**
- 10:15 - 10:40 **Ivan Shabalin, PhD - University of Virginia**
"Reliability of Protein Crystal Structures for Structure-based Drug Discovery."
- 10:40 - 11:05 **Banu Ozkan, PhD - Arizona State University**
- 11:05 - 11:30 **Vasant Honavar, PhD - Pennsylvania State University**
- 11:30 - 11:55 **Gabriel del Rio, PhD - Universidad Nacional Autonoma de Mexico**
"Designing Polypharmacological Polypeptides: From Single and Unifunctional Targets to Multifunctional Drugs"
- 11:55 - 1:40 **LUNCH & FREE TIME** (Optional - "Writing Grant Proposals")

HOST PATHOGEN INTERACTIONS - Chair: Faeder

- 1:40 - 2:25 **Arup Chakraborty, PhD - Massachusetts Institute of Technology (MIT)**
- 2:25 - 2:55 **James Faeder, PhD - University of Pittsburgh**
"Determining the Role of T Cell Antigen Receptor Signaling Strength in T Cell Differentiation"
- 2:55 - 3:25 **Elizabeth Read, PhD - University of California, Irvine**
- 3:25 - 3:40 **BREAK**
- 3:40 - 4:10 **Elsje Pienaar, PhD - University of Michigan**
"Mapping Mycobacterial Metabolic Scale Perturbations to Tissue Scale Outcomes in Tuberculosis"
- 4:10 - 4:40 **Jayajit Das, PhD - Nationwide Children's Hospital**
- 4:40 - 5:45 **Transportation to Nationwide Children's Hospital via charter bus**
- 5:45 - 6:30 **Poster Session**
- 6:30 - 8:30 **Gala Dinner**

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Mathematical and Computational Medicine**

Wednesday, May 18, 2016

Day 3

8:30-9:15

Keynote Speaker

Philip Bourne, PhD - National Institutes of Health

"Big Data in Biomedicine – Has Anything Fundamentally Changed?"

INFERENCE, EVIDENCE & ENTROPY - Chair: Presse

9:15 - 9:55

Steve Frank, PhD - University of California, Irvine

"Measurement Scale and Dissipation of Information Shape Biological Pattern."

9:55 - 10:20

Steve Presse, PhD - Indiana University Purdue University Indianapolis

"Inference from Imaging Data"

10:20 - 10:45

David Bickel, PhD - University of Ottawa

"Inference Under the Entropy-Maximizing Bayesian Model of Sufficient Evidence"

10:45 - 11:00

BREAK

11:00 - 11:25

William Stewart, PhD - Nationwide Children's Hospital

11:25 - 11:50

Veronica Vieland, PhD - Nationwide Children's Hospital

"How to Know When We Are (or Are Not) Measuring Statistical Evidence"

11:50 - 1:45

LUNCH & FREE TIME

Founding Society for Mathematical and Computational Medicine Business Meeting

Lunch Included

VISUALIZATION - Chair: Ray

1:45 - 2:30

Gael McGill, PhD - Harvard University

"Exploring Hollywood's Tools for Biovisualization: Data Exploration, Working Models and Communication"

2:30 - 3:00

Paul O'Mallie, PhD - Norwich Research Park, UK

"Unraveling a Half-Century Old Mystery: Elucidating Drug Mechanism of Action with Metabolomics."

3:00 - 3:30

Hamid Younesy, PhD - Simon Fraser University

3:30 - 4:00

Irina Buhimschi, MD - Nationwide Children's Hospital

4:00

CLOSING REMARKS & ADJOURN