www.ietdl.org

Published in IET Systems Biology doi: 10.1049/iet-syb.2010.9133

Special issue on the Third *q-bio* Conference on Cellular Information Processing

Editorial

The Third *q-bio* Conference on Cellular Information Processing

Summary: This Special Issue consists of 11 original papers that elaborate on work presented at *The Third q-bio Conference on Cellular Information Processing*, which was held on the campus of St. John's College in Santa Fe, New Mexico, USA, 5–9 August 2009.

The q-bio Conference has marked its third anniversary (in fact, as we are writing this, the fourth installment of the conference has concluded, the discussion of which is for the next Special Issue). It is fair to say that, in the three years since the inaugural event, the conference has established itself as a prominent meeting on the landscape of international systems biology gatherings. The conference fills an important gap in the field through its emphasis on quantitative, predictive modelling, high precision, physics-style experimentation, and theoretical quest for general principles of biological design. This year we began to see the students and postdocs of those who had presented at the earlier q-bio events, providing a glimpse of the impact of the conference on the community. The number of students at the affiliated *q-bio* summer school increased again; and attendance at the conference remained high despite the tough financial times. The 2009 conference attracted prominent biologists such as Bruce Alberts, Rita Colwell, and Michael Levin and it was encouraging to see these representatives of 'traditional' biology embrace the spirit of the meeting and the emerging field. The conference and the field owe Dr. Colwell a debt of gratitude, as her tenure as Director of the National Science Foundation is widely credited with the explosive growth of quantitative techniques in the life sciences - techniques without which q-bio science would be impossible.

This year the National Institute of General Medical Sciences (NIGMS) provided funding for nearly 100 travel awards that helped bring junior researchers to the event. As a result, the conference grew to include 27 invited talks, 22 contributed talks (twice as many as the year before!), 16 poster spotlights, and 110 contributed poster presentations (again, a record!). Over three quarters of all of the conference attendees presented, helping to sustain the uniquely dynamic and engaging atmosphere of the q-bio conference.

What's next for q-bio? There has been a significant investment in systems biology recently. For example, in the United States, there is now a network of National Cancer Institute (NCI) supported Cancer Systems Biology centers, a network of NCI-supported Physical Science-Oncology Centers, and a network of NIGMS-supported Systems Biology centers, all of which, clearly, explore quantitative and systems approaches to cellular regulatory processes. These investments signal a growing need for modelling and theory - the hallmarks of q-bio. But where will the modellers, theorists and quantitative experimentalists come from? As an event targeted towards early career scientists, with an affiliated summer school, q-bio is helping to create new communities of researchers that will fill the ranks. As a relatively small, agile event, it is also positioned to respond to the newly opening directions in systems biology, such as a merger of population biology, ecology and evolution with molecular and cellular biology and the newest biotechnology, where quantitative, systems approaches serve as glue. In short: the future is bright for q-bio! And, as organisers, we intend to keep it an event that breaks the frontiers of biology. The Fifth q-bio Conference is scheduled for August 10-13, 2011, in Santa Fe, New Mexico, USA with satellite meetings on August 14. The Fifth q-bio Summer School will open its doors on July 25, 2011. We will see you there!

The Special Issue at a Glance

As in previous years, the Special Issue is a snapshot of presentations at the q-bio. Even though the conference



itself is almost equally split between computational and experimental contributions, the Special Issue is tilted towards theory and computation. It remains a challenge to recruit experimental contributions to the issue.

The eleven individual papers in this Special Issue speak for themselves. We encourage readers to inspect them directly, and the introductions below are deliberately brief. We have arranged the papers loosely into three themes: *Modelling*, *Theory*, and *Tools*.

Modelling: This section consists of four papers devoted to models of specific cellular systems. It starts with the work by Goldstein and co-workers, who continue their longterm program of developing a detailed mathematical model of events in IgE receptor signalling. Lipniacki and coworkers present a model of spatially-resolved kinase signalling in Spatial Gradients in Kinase Cascade Regulation to investigate effects of spatial dynamics of receptors on sensitivity to signals. This paper is followed by the contribution of Munsky, who presents a stochastic model of a synthetic genetic switch and investigates the conditions under which parameters of the system can be inferred from experiments. Finally, the section ends with a study of a biophysical model of cargo delivery through a cell membrane in the paper Cell-Penetrating Peptides, Electroporation, and Drug Delivery by Cahill.

Theory: Papers in this section focus on general properties of molecular networks that transcend specific modelling examples. Maienschein-Cline *et al.* (*Defining cooperativity in gene regulation locally through intrinsic noise*) and Igoshin and Narula (*Thermodynamic models of combinatorial gene regulation by distant regulatory elements*) independently explore different mechanisms for generation and approaches for analysis of combinatorial, cooperative transcriptional regulation. In the third paper of this section, Sinitsyn and Nemenman analyse effects that time dependence in kinetic parameters of a Michaelis-Menten reaction may have on experimentally observable molecular fluxes.

Tools: The four papers in this section describe computational and experimental tools for inference and simulation of biochemical reaction networks. The first paper (Enders et al.) presents an experimental platform that blends microfluidics with ion-mobility mass spectrometry for high-throughput real time profiling of cellular metabolic and protein states. The paper by Margolin et al., presents a systematic definition of a statistical dependency in a multivariate context and uses the definition as the basis for an algorithm for reverse-engineering of cellular regulatory networks from high-throughput profiling data. Finally, the last two papers, Wolf et al., and Yang et al., explore computational techniques for solution of the chemical master equation that underlies stochastic biochemical processes using complementary numerical integration and kinetic Monte Carlo approaches.

Acknowledgments

We thank the authors who contributed to this Special Issue and the over 25 anonymous reviewers of manuscripts, as well as the staff of IET Systems Biology for their continued support of q-bio. Additionally, we would like to thank the staff of St. John's College Conference Services and the staff of the Center for Nonlinear Studies and the Theoretical Biology and Biophysics Group in Los Alamos, especially Jenny Esch, Adam Shipman, Don Thompson, and Ellie Vigil. We also thank the Center for Nonlinear Studies and the Institute for Advanced Studies at Los Alamos National Laboratory, the NIGMS-funded Center for the Spatiotemporal Modelling of Cell Signalling at the University of New Mexico, the New Mexico Consortium, Plectix BioSystems, the Emory University Computational and Life Sciences Strategic Initiative, and NIGMS (NIH grant GM082162) for generous financial support. We also thank the many invited speakers who declined travel support so that more funds could be used to help junior researchers participate in the meeting. Finally, we thank the advisory and program committee members, who helped the organisers assemble the program, recruit speakers, review submitted abstracts and publicise the event: Blagoy Blagoev (University of Southern Denmark), Naama Brenner (Technion), Thierry Emonet (Yale University), James R. Faeder (University of Pittsburgh School of Medicine), Alexander Hoffmann (University of California, San Diego), Orna Resnekov (Molecular Sciences Institute), Thomas S. Shimizu, (FOM Institute for Atomic and Molecular Physics), Robert H. Austin (Princeton University), Roger Brent (Molecular Sciences Institute), Hans Frauenfelder (Los Alamos National Laboratory), Byron Goldstein (Los Alamos National Laboratory), Dale Kaiser (Stanford University), Keiichi Namba (Osaka University), Janet M. Oliver (University of New Mexico School of Medicine), Bernhard Ø. Palsson (University of California, San Diego), Thomas D. Pollard (Yale University), John Reinitz (Stony Brook University), Michael A. Savageau (University of California, Davis), and Thomas C. Terwilliger (Los Alamos National Laboratory).

The organisers of *The Third q-bio Conference and Summer School* and the editors of this Special Issue are:

> ILYA NEMENMAN WILLIAM S. HLAVACEK YI JIANG MICHAEL E. WALL ANTON ZILMAN

(Atlanta, Georgia; Los Alamos, New Mexico; and Scottsdale, Arizona; October 2010)

Dr Ilya Nemenman received a PhD in theoretical physics from Princeton University. He trained as a postdoctoral scientist at the NEC Research Institute and the Kavli Institute for Theoretical Physics, and as an Associate Research Scientist at the Columbia University School of Medicine. He was a staff scientist at Los Alamos National Laboratory before joining Emory University Departments of Physics and Biology, where he studies information processing in biological systems.

Dr William S. Hlavacek received a PhD in chemical engineering from the University of Michigan and did postdoctoral work at Los Alamos National Laboratory, where he is now a Scientist in the Theoretical Division. He is also a Research Associate Professor in the Department of Biology at the University of New Mexico. He has worked on modelling bacterial gene regulation, metabolic networks, multivalent ligand-receptor binding, HIV dynamics, and signal transduction in cancer and immunity. He is currently on sabbatical at the Translational Genomics Research Institute, where he is the Visiting Pausch Scholar.

Dr Yi Jiang received her PhD in physics from University of Notre Dame and was a postdoc at Los Alamos National Laboratory before she became a staff scientist at the Theoretical Division, where she has been since. She is also an Adjunct Professor at Mathematics Department of Notre Dame and Physics Department at Emory. She has broad interests in biophysics, from complex fluid rheology, macromolecular assembly, to tissue morphogenesis. Her Recent research is focused on cancer development, bacterial patterning, and cellular networks.

Dr Michael E. Wall is a staff scientist in the Computer, Computational, and Statistical Sciences Division at Los Alamos National Laboratory, where he is also affiliated with the Bioscience Division and the Center for Nonlinear Studies. Dr. Wall's training is in experimental biophysics, biochemistry, and computational biology. His work has addressed problems in protein function and dynamics, diffuse scattering, small-angle scattering and gene regulation. He is generally interested in theoretical and computational modelling of biochemical regulation.

Dr. Anton Zilman is a J. Robert Oppenheimer Distinguished Postdoctoral Fellow at Los Alamos National Laboratory. He has been trained as a theoretical biophysicist in Tel Aviv University and Weizmann Institute. He joined Los Alamos after a postdoctoral appointment at The Rockefeller University. His research interests span a broad range of topic including theoretical immunology and biomolecular transport. In January 2011, Dr. Zilman will join the Department of Physics at the University of Toronto as an Assistant Professor.