Computational Biology: Its Challenges Past, Present, and Future

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Dedication: To a friend and inspiration, Stanislaw Ulam.

I was lucky not only to have known Stan (Dr. Ulam), but to have been befriended by him. I would note that it was with his support that my first "computational" biology paper was published and that I was then a physics graduate student who had not taken or read biology since the sixth grade! I will outline just a few Ulam anecdotes in his memory.

Abstract. The recognition of the role of mathematics and computer science in modern biology has led to new terminology, as did chemistry with biochemistry, and physics with biophysics. We need to think only of bioinformatics, computational biology, and even system biology and genomics for example. These terms seem to strongly suggest that this is all rather new. Yet a short review of the work of those such as J.B.S. Haldane, Sewell Wright, DArcy Thompson and R.A. Fisher, to say nothing of scientists like Luria and Delbrueck or Hodgkin and Huxley or Thomas Hunt Morgan, is useful. Their work and foresight set the stage for modern applications of mathematical modeling and statistics in the biological sciences.

It has often been said that the only difference between now and then is the increase in data—a lot more data. This is clearly not the full story. In addition, we have computational power unimaginable to these earlier researchers, as well as to anyone only forty years ago. So what are our challenges? Some are clear, including the modeling and analysis of biologys complex systems such as a cells signaling, metabolic and differentiation. Also needed are analysis and models of complex neural systems and ecological structures. The latter, for example, will require a nearly full revamping of the early field of population genetics and evolution in order to exploit both modern genomics and new field studies of multiple species and environmental interactions. And there will be more, much of which will only become apparent as new data and questions arise. One example would be RNAi and micro-arrays inducing the development of new analysis tools.

About the keynote speaker. Dr. Temple Smith graduated with a Ph.D. in Nuclear Physics from University of Colorado. He did a joint postdoctoral fellowship under the direction of the mathematician, Stanislaw Ulam and the molecular biologist, John Sadler. He was one of the founders of GenBank at Los Alamos. Dr. Smith has been the Director of the BioMolecular Engineering Research Center in the College of

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Engineering at Boston University since 1991. He is a professor in the Department of Biomedical Engineering and co-founder of the company, Modular Genetics, Inc.

Dr. Smith is a co-developer of the Smith-Waterman sequence alignment algorithm, the standard tool used in most DNA and protein sequence comparison. His research is centered on the application of various computer science and mathematical methods to the discovery of the syntactic and semantic patterns in nucleic acid and amino acid sequences. These include the development of new sequence pattern extraction tools, multidomain dissection methods, and protein inverse folding prediction algorithms. In addition, Dr. Smith has carried out research in the application of many such methods ranging from the time calibration of HIV viral evolution analysis and modeling of the WD repeat family of proteins, to ribosomal protein evolution.