ABME Special Issue: Systems Biology, Bioinformatics, and Computational Biology

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This special issue consists of a wide range of articles that are related to presentations in the Systems Biology & Bioinformatics (SB&B) track of the 2006 Annual Meeting of the Biomedical Engineering Society. We believe that the SB&B field is now exploding with opportunities for bioengineers and biomedical engineers to implement many aspects of computational analysis of biological systems from the molecular level to the whole organism. The scope of SB&B analysis encompasses computational biology involving modeling or algorithmic methods for quantitative analysis of complex biological systems. Usually, its central focus is to quantify processes at the molecular and/or cellular level. Often, the analysis depends on extensive experimental datasets.

Systems biology can be distinguished by its intention to quantitatively explain and predict molecular, cellular, tissue, organ, and whole body processes. For this purpose, computational models are developed to analyze multi-variable, multi-scale, and large-scale systems based on underlying physical and chemical processes. These computational models emphasize biological phenomena at the cellular level. When applied to human health, systems biology models are intended to predict physiological behavior in response to natural and artificial perturbations. Consequently, the models can be used to quantify normal and abnormal function that can lead to the development of diagnostic and therapeutic methods for human disease.

Bioinformatics describes a field that deciphers information contained in the genetic blue print of life through discovery of genes, inference of the structure and function of gene-encoded proteins and RNAs. It provides a quantitative analysis of the expression patterns of genes and proteins, and how such expressions are regulated in different tissues and organs. This rich information ultimately leads to better understanding of the health state of cells and the mechanisms of disease genesis. Practical applications include engineering of modified proteins with improved properties, development of therapeutic interventions, and quantitative diagnosis and prognosis of diseases.

The articles in this issue deal with a variety of methods and applications that are described briefly here. In the first two articles of the nine that relate to systems biology, analyses of large-scale system models of metabolism incorporate optimization and statistical methods. Statistical methods are also applied with stochastic modeling of cell population dynamics to cancer treatment. Models of multi-cell dynamics that involve molecular mediators and cell trafficking provide quantitative understanding of processes in the microvasculature and lung. Multi-scale models that relate changes in tissues to cellular processes associated with key molecular species are applied to analyze changes in the microvasculature and metabolism of muscle in relation to exercise. Network models are presented that examine intra-ovarian metabolism and actin regulatory mechanism in cells.

The last nine articles are representative of bioinformatics and molecular computational biology. These deal with molecular dynamics and computational docking applied to dissect early events in signal transduction. Molecular modeling also allows engineering of interfacial pockets on protein molecules with modified substrate binding properties. Effective computational methods for identifying substrate binding sites from enzyme structures are also reported. Novel tools for identifying proteins binding to DNA and membranes are presented, which include transcription factors, an important class of proteins regulating various cellular processes. Systematic automated high-throughput analyses of subcellular locations of proteins are applied to large sets of microscopic images. The differential expression levels of genes in different tissues are correlated with their

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cellular roles. An optimization-based machine learning approach is developed to identify disease states and predict prognosis outcomes for a number of important diseases.

We expect that systems biology, bioinformatics, and computational biology will continue to blossom with key contributions from bioengineers and biomedical engineers.