Preface

Dagstuhl Seminar on Integrative Bioinformatics

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Molecular biology produces huge amounts of data in the post-genomic era. Among them, there are data describing metabolic mechanisms and pathways, structural genomic organization, patterns of regulatory regions, proteomics, transcriptomics and metabolomics data. On one hand, analysis of these data is determined essentially by the methods and concepts of computer science, on the other hand, it depends on a range of biological tasks solved by researchers. Currently, there are about 600 database information systems and various analytical tools available via the Internet. The challenge we have is to integrate these software tools from genomics and proteomics at novel levels of understanding. Integrative Bioinformatics would be this new area of research using the tools of computer science and electronic infrastructure applied to biotechnology. These tools also represent the backbone of the concept of the Virtual Cell, which was the scientific topic of the Dagstuhl Seminar on Integrative Bioinformatics: Aspects of the Virtual Cell 2004. The Seminar addressed primarily scientists working in this emerging field of Integrative Bioinformatics and, hence, discussed the corresponding problems and presented concepts. Consequently, the topics of the Seminar covered data integration, method integration and a combination of both as well as applications of theoretical /computational tools and any other approach supporting an integrative view on metabolic systems.

The seminar was organized by J. Collado-Vides (UNAM Mexico), C. Sensen (University of Calgary) and R. Hofestädt (Bielefeld University). First, a number of talks were presented that dealt with molecular database systems and integration tools. The second topic of the seminar was integrative modeling of signal transduction, gene regulation and metabolic events. Cell modeling, visualization and animation of metabolic processes was the third topic.

This special issue represents selected papers of the Dagstuhl seminar. These papers show that Bioinformatics is using methods of integration to start the discussion and implementation of aspects of the Virtual Cell. Using molecular data and knowledge, which is available via the Internet, the implementation of cellular models allows the implementation of simulation tools. Behind the algorithmic analysis of molecular data, modeling and simulation methods and concepts allow the analysis and synthesis of complex gene controlled metabolic networks. Today the molecular knowledge is still rudimentary. Therefore, methods of modeling and simulation will help to understand many important scientific questions. Such formal

descriptions can be used to specify a simulation environment. Therefore, modeling and simulation can be interpreted as the basic step for implementatiing virtual worlds that allow virtual experiments. Behind the discussion of databases and integration tools it was one important part of the seminar to discuss the Petri net formalization for the modeling of metabolic networks.

The presented papers show parts of the electronical infrastructure of the Virtual Cell and the application of molecular data to model and simulate metabolic processes. To solve current questions in the field of the Virtual Cell, we have to implement integrative models. If we take a look to the Internet, we can see that online representations of cellular representations are available. Also the well-known E-cell system of M. Tomita represents a specific software solution, which cannot be used as a global implementation of a Virtual Cell (www.e-cell.org). Different new Virtual Cell projects are running all over the whole world. However, it will take a lot of time to implement an useful and powerful implementation. Rudimentary knowledge is the main problem. That means, we are still not able to understand the quantitative behavior of simple metabolic processes.

We would like to thank Schloss Dagstuhl International Conference and Research Center for Computer Science for accepting our proposal. The Dagstuhl Seminar Integrative Bioinformatics – Aspects of the Virtual Cell, which was held in Dagstuhl July 2004, was the fourth Dagstuhl Seminar of Modeling Metabolic Networks (1995, 1998 and 2001). The next seminar about this topic is planned for July 2007.

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