The problem of using current data with a state model of cell signaling molecules was discussed by Shankar Subramanian, University of California, San Diego (http://www.ucsd.edu). Igor Goryanin, GlaxoSmithKline, gave an overview of the field of whole-cell modeling, and spoke of his group's efforts to model *Escherichia coli* and the potential pharmaceutical applications of this project.

Mathematical models

One of the major differences in opinion of the speakers was what sort of mathematical model to use. Some use differential equations, others use discrete methods, still others use probability theory and statistics and some use hybrid mathematical models combining continuous ordinary differential equations with discrete cellular automata models. To those not familiar with mathematics, it is similar to mixing oil and water; discrete and continuous models are based on different mathematical foundations. However, such a hybrid approach, even if not mathematically clean, might help in understanding complex data. The problem is how to relate the two models in a way that maintains both scientific rigour and the ability to explain and predict phenomena.

In the session on Target Prioritization and Drug Development, Tom Paterson, Entelos (http://www.entelos.com), presented the Virtual Patients framework, which, he claimed, will allow the testing of drugs *in silico* and *in silico* predictions of drug interactions. Bernard Palsson asked a provocative question: What is a pathway for you? The answer illuminated the fact that Entelos seems to have broadened the definition of a pathway by allowing pathways that directly relate low-level molecular interaction with high-level biological phenomena, such as a phenotypic property of a cell or even the effects on the morphology of an organism. This makes it clear that such pathways or networks are hybrid constructions, which is something that mathematical purists might view sceptically. Furthermore, it could make the relationship between the model and the data an *ad hoc* construction. This could lessen if not negate the explanatory and predictive power of the model. By contrast, if done correctly, it could give such models new integrative and predictive power. For sometimes the mathematics has to be developed to fit reality, rather than the other way around.

Christos Hatzis, Silico Insights (http://www.silicoinsights.com/), discussed the problem of integrating data from different levels of organizations. In particular, his company addresses the problem of integrating prior knowledge of genes with experimental measurements of gene expression with the aim of elucidating function. His point was emphasized by several speakers who spoke of the value of preexisting literature on genes in understanding the function of genes and gene expression data.

Summary

Overall the conference showed that systems biology is not only off to a good start but beginning to take off into a promising and exciting future. The movement from wet lab to *in silico* experiments, could not only speed up research and reduce the enormous costs of drug development, they could redefine the very foundations of biology. No longer can a biologist ignore computer science and mathematics. They are becoming an essential component of the field. At the same time the student might benefit if software provides a release from the endless hours, months and years of laboratory work now required to do wet lab experiments. Indeed, the integration of computer science and biology could change our world as much as the computer changed our world in the past century.

Erratum

Please note a correction to the article Tailoring vaccines to individual lymphomas by Matt Brown, published in *Drug Discovery Today*, 1st July 2002, Volume 7, No. 13, 693–694.

We incorrectly stated that a team led by Aaron Rapoport at the University of Maryland had developed the vaccine to treat follicular lymphoma, when in fact the vaccine was invented by Ronald Levy at Stanford University but is being trialed by Rapoport's team against non-Hodgkin's lymphoma.
We would like to apologize for this inaccuracy and for any misunderstanding that this might have caused.

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