

## **3<sup>rd</sup> Genomics-Bioinformatics Day: "Bioinformatics, Computational Biology, Systems Biology & Mathematical Biology: Their Relationship" October Thursday 1PM April 29<sup>th</sup> 2003 at Oxford Centre for Gene Function, 3<sup>rd</sup> floor.**

April 24<sup>th</sup> and October 7<sup>th</sup> we had very successful days on "Comparative Genomics" and "Analysis of Pathogens", respectively, that brought together researchers within Oxford. It caused a lot of exchange of ideas and awareness of common interests and possibilities for collaboration.

We will now continue this tradition with a day arranged by Jotun Hein, Santiago Schnell and Philip Maini with the focus on "Bioinformatics, Computational Biology, Systems Biology & Mathematical Biology: Their Relationship". Genomics, Bioinformatics, Computational Biology have a tremendous appeal and these fields have originated or grown enormously during the last 5-10 years. Systems Biology and Mathematical Biology are also growing rapidly, but having a longer scientific history. Despite the present popularity of the new comers, it seems that Modelling in Biology will be increasingly in demand in coming years. Are these fields distinct? If distinct, which collaborative efforts would be most fruitful? Will their relative importance in the Bioscience change in coming years?

It is our intention to have such a half day beginning of each term. The day will be dedicated to an interesting topic and will also be used to announce Genomics/Bioinformatics in the following term: seminars, study group and other meetings. A topic for the next half day could be "Expression Data and Bioinformatics" in beginning of Michalmas Term.

In case you plan to attend this event, please email (Victoria Hansford) [hansford@stats.ox.ac.uk](mailto:hansford@stats.ox.ac.uk) so coffee and tea can be made accordingly. If you cannot enter OCGF directly, you can through the Physiology Building.

### **General Considerations 1.00-1.30PM**

#### **Hein & Schnell: Introduction: Mathematical Biology and Bioinformatics.**

Both Bioinformatics and Mathematical Biology have been developing fast in recent years. Bioinformatics has diversified and moved "beyond sequences and genomes". Mathematical Biology has become central in the analysis of new data types from diverse newly arisen (or at least named) "-omics" fields such as expressionomics, metabolomics,.. What are the differences and commonalities between Mathematical Biology and Bioinformatics. Recent post-genomic bioinformatics have seen much research that involves modelling biological systems and subsequent inference of biological structures such as regulatory paths. Much large scale modelling uses ontologies, functional annotation of genes and activities that would normally be seen as bioinformatics.

### **1.30-2.30PM Networks and Metabolic Pathways**

1.30 – 1.50 Mark Poolman (Oxford Brookes University)

#### **"Structural analysis of metabolic systems: from pathways to genomic scale"**

Biochemical models are defined by lists of reactions supplemented by auxiliary information. The information that can be extracted from such models is thus dependent on the information used to define the reactions. In this talk, the utility of models based on the minimal information, the stoichiometric equation for each reaction of the network, is illustrated with reference to small metabolic systems. The challenges in extending this approach to genomic scale models will be discussed.

1.50 - 2.10 David Fell (Oxford Brookes University)

### **"Building kinetic models of metabolism"**

A case study of threonine metabolism in *E. coli* will be used to illustrate the issues arising in constructing a kinetic model even for well-known reactions in a much-studied organism. For example, even though the kinetic properties of the individual enzymes have been extensively researched, the results are often not appropriate for use in representing metabolism *in vivo*. Although it proved possible to gain useful insights from a working model of this section of metabolism, the amount of experimental effort required shows that there is a bioinformatic gap before genomic scale kinetic models can be contemplated.

### 2.10-2.30 Herbert Sauro (Cal Tech) **"Modularity in signaling networks"**

In this talk I will discuss some aspects of modularity in biochemical networks. In particular I will discuss the MAPK and chemotaxis models as examples of modules. Lastly an evolutionary approach will be discussed as a means to uncovering more motifs and to begin the task of building a circuit theory for signaling networks.

### **Coffee Break 2.30PM-3.00 PM**

### **3.00-4.20 PM Multiscale Modelling**

Denis Noble **"What does computational biology try to achieve?"**

Computational biology will find it difficult or impossible to achieve its goals through bottom-up reconstruction or through purely top-down analysis. I will illustrate what Sydney Brenner called the middle-out approach, using heart models as an example.

David Gavaghan: **The Integrative Biology e-Science Project**

This project aims to build the computational infrastructure for the *in-silico* modelling of complex biological systems. I will give a (very brief) overview of the project objectives.

Alan Garny: **Multicellular computer models of the origin and spread of cardiac excitation**

Models of the rabbit sino-atrial node were developed to study how cardiac activity originates and spreads into the atrium. These models make use of cellular models that describe the electrophysiological behaviour of various cardiac cell types. Anatomical information on the sino-atrial node region and its atrial surroundings have also been included in some of the models.

### **4.20- General Discussion** – moderator Philip Maini