ICSB 2013 Copenhagen

Workshop and Tutorial schedules Location DTU, about 15 km north of Copenhagen Times are approximate

Thursday, August 29

9.00 – 17.00 DTU meeting center, room 1 The Virtual Liver: a multidisciplinary, multilevel challenge for Systems Biology Adriano M Henney, Johannes Bausch

9.00 – 18.00 DTU meeting center, room 5 **Garuda Workshop**

Hiroaki Kitano, Samik Ghosh, Yukiko Matsuoka, Nikos Tsorman

9.00 – 18.00 DTU meeting center, room S01 Understanding Biological Processes using PathVisio and Cytoscape.

Susan Coort, Martina Kutmon, Thomas Kelder

9.00 – 13.00 DTU meeting center, room S09 **DNAdigest: translational genomics - from bioinformatics to medical informatics**Fiona Nielsen, Søren Brunak, Jennifer Becq, Mette Nyegaard

9.00 – 18.00 DTU meeting center, room 4 Experimental data and metadata management

Dalibor Štys, Petr Císař, Jan Urban, Renata Rychtáriková, Aliaxander Pautsina, Tomáš Náhlík, Anna Zhyrova, Karina Romanova and Rebecca Smaha

Friday, August 30

9.00 – 13.00 DTU meeting center, room 5

Experimental data and metadata

management - continued

Please find the abstracts below.

9.00 – 13.00 DTU meeting center, room 2 **GenoCAD Tutorial**

Jean Peccoud

Tuesday, September 3

14.00 – 17.00 DTU meeting center, room 1 CASyM workshop: Should systems medical training be integrated for basic and clinical researchers?

Mikael Benson, Mika Gustaffson, Marc Kirschner, Hans Westerhoff, Gerold Baier, Charles Auffray, David Harryson, Damjana Rozman

14.00 – 18.00 DTU meeting center, S02/S12 AllBio workshop on Standardisation Operation Procedures (SOP)

Susanne Hollmann, Babette Regierer, Joachim Lonien, Martin Golebiewski

Wednesday, September 4

9.30 – 17.30 DTU meeting center, room 1

Tutorial: Modelling and Simulation of Quantitative Biological Models

Martin Golebiewski, Frank Bergmann, Akira Funahashi, Noriko Hiroi, Mike Hucka, Nicolas Le Novère, Pedro Mendes, Ion Moraru, Sven Sahle, Jacky Snoep, Dawie van Niekerk, Andreas Weidemann, Katy Wolstencroft

The Virtual Liver: a multidisciplinary, multilevel challenge for Systems Biology

Adriano M Henney, Johannes Bausch

The Virtual Liver: a multidisciplinary, multilevel challenge for Systems Biology The Virtual Liver Network is a Flagship Research Programme funded by the German Government focusing on work at the "bleeding edge" of systems biology and systems medicine. It aims to tackle a major challenge in the life sciences: how to integrate the wealth of data we have acquired post-genome, not just in a mathematical model, but more importantly in a series of models that are linked across scales to represent organ function. The liver is the central metabolic organ in human physiology, with functions that are fundamentally important to the detoxification of xenobiotics, the maintenance of homeostasis and the production of mediators of the acute phase response. Liver toxicity, whether actual or implied is the reason for the failure of a significant proportion of many promising novel medicines that consequently never reach the market. The workshop will be structured around the four showcase studies that are the central themes of the integrated work plan in the network, which address regeneration, inflammation, steatosis and the effects of biliary flow. The approach will combine invited oral presentations, posters and discussion groups around the challenge of translating the work at the bench into the clinic. A key aim is to engage industry in evaluating the potential to use the experiences, skills and knowledge gained in the VLN to support the development of systems pharmacology and predictive toxicity tools for drug discovery.

Garuda Workshop

Hiroaki Kitano, Samik Ghosh, Yukiko Matsuoka, Nikos Tsorman

The rapid development of high throughput experimental techniques is transforming life science research. Software for biomedical research forms a critical component for success – to aggregate, analyze and interpret the heterogeneous data in a systems-level context. While various software tools individually provide specific analytical functions, each operates on unique inut/outputs, graphical interfaces and workflows. The lack of inter-operability and data sharing leads to extra work for developers and users.

The goal of the Garuda project is to develop an open, common platform for biomedical research, providing consistent and zero-configuration user experience and easy-to-use programming interfaces. The Garuda Alliance endeavors to provide a one-stop shop for researchers in academics and pharmaceutical industry sectors. Launched by The Systems Biology Institute, Japan, Garuda Alliance members currently include global leaders in systems biology tools and databases like CellDesigner, Physiodesigner, Cytoscape, Reactome, to name a few.

The computational framework is developed around the central platform modules (Garuda Core), Garuda API (set of programming interfaces to enable development of software modules known as Garuda Gadgets) and Garuda Dashboard (provides the user interfaces to interact with Garuda). The framework is language, tool or format agnostic. With the Garuda platform, academic community and industries do not have to re-invent similar tools with only minor variance. Third parties can invest their resources to develop gadgets and software tools without worrying about compatibility and sustainability of the platform.

The goal of the workshop is to introduce the Garuda Platform (beta) to the larger community of researchers attending ICSB2014 and demonstrate how Garuda enables them to discover and seamlessly integrate various tools and services in their research workflows.

The tentative sessions for the workshop would aim to initiate users through the overview overview (Hiroaki Kitano), platform overview and demo(Samik Ghosh), user perspectives (Yukiko Matsuoka) and developer perspective and hand-ons (Nikos Tsorman).

Understanding Biological Processes using PathVisio and Cytoscape.

Susan Coort, Martina Kutmon, Thomas Kelder

Biological processes consist of information on genes, proteins, metabolites, interactions. Nowadays it is possible to measure the biomolecules on a large scale generating enormous amounts of data. In addition, regulatory mechanisms by for example microRNAs and epigenetic modifications are being deciphered. Although this gives researchers new insights, it makes the system more complex. Tools and methods to analyze these complex regulatory processes should be developed and used in a sophisticated way to interpret the biological meaning. Open-source projects like WikiPathways, PathVisio and Cytoscape, are important tools for advanced analysis of biological processes. Our workshop fits well with the sessions on i) Metagenomics, ii) Genetic networks, iii) Metabolomics, iv) Protein interactions networks and v) Signalling networks. All co-chairs are actively involved in development communities of the tools demonstrated in the workshop and can provide in-depth explanations to the participants. Each co-chair applies these tools in different areas of research, such as nutrition and cardiology (Susan Coort), toxicology (Martina Kutmon), and metabolic health and microbiology (Thomas Kelder).

Note: Participants should bring their own laptops.

DNA digest: translational genomics - from bioinformatics to medical informatics

Fiona Nielsen, Søren Brunak, Jennifer Becq, Mette Nyegaard

In this workshop we will present the current challenges in translational genomics. We will discuss how research findings in genomics can be linked to and have an impact for medical diagnostics.

Four presentations will cover the views from bioinformatics to medical genetics. There will be time set aside for Q&A with our presenters, and we will encourage you to participate in the discussion.

Søren Brunak, Professor, Center for Biological Sequence Analysis:

Data mining medical records for new insights for diagnostics

Jennifer Becq, Bioinformatics Scientist, illumina Cambridge:

From sequencing a tumour sample to finding actionable variants

Mette Nyegaard, Associate Professor Human Genetics, Aarhus University:

A novel deafness locus and gene mutation on chromosome 6q15-q21 identified using linkage analysis and next generation sequencing

Fiona Nielsen. co-founder DNAdigest.org:

Protecting data and sharing knowledge - Enabling secure data access for advancement of genomics research

Host: Fiona Nielsen, DNAdigest.org

DNAdigest is a not-for-profit organisation founded for the purpose of solving the problem of sharing genomics data for research purposes. DNAdigest presents a secure mechanism for publishing genome data, which would otherwise not be shared with the broader research community. Read more and sign up for our newsletter at http://DNAdigest.org.

Experimental data and metadata management

Dalibor Štys, Petr Císař, Jan Urban, Renata Rychtáriková, Aliaxander Pautsina, Tomáš Náhlík, Anna Zhyrova, Karina Romanova and Rebecca Smaha

The first part of the workshop is going to present the solution in the field of experimental data and metadata management. The solution is developed in the frame of the BioWes (www.biowes.com) project and tries to cover all aspects of data management, including experimental and data analysis protocols. The general philosophy of the project is an assumption that the plan of the experiment is based on extended background information which is not fully intelligible from the resulting dataset. The aim of the workshop is to introduce the solution for experimental data and metadata standardization, storage, and sharing along with the tools for data processing.

The second part of the workshop will discuss the data processing and analysis of mass spectrometry measurements based on a probabilistic approach, automation of the steps, and interpretation of the confidence level.

In the third part of the workshop, the participant will present their own contribution to the workshop topics.

There will be also a publication opportunity in a special issue of International Journal of Molecular Sciences (IF 2011 =2.598).

GenoCAD Tutorial

Jean Peccoud

Systems and synthetic biology are cross-fertilizing each other in unexpected but very productive ways. For several years ICSB has included synthetic biology sessions. Many keynote speakers are known for their work in synthetic biology or at the interface between synthetic and systems biology. This tutorial will give ICSB participant an opportunity to practice synthetic biology in a classroom environment using GenoCAD, an open source web-based system that provides a streamlined, rule-driven process for designing plasmids, gene expression systems, or artificial gene networks. GenoCAD provides a graphical interface allowing users to design sequences consistent with formalized strategies specific to a domain, organization, or project. Design strategies include limited sets of user-defined parts and rules indicating how these parts are to be combined in genetic constructs. In addition to reducing design time to minutes, GenoCAD improves the quality and reliability of the finished sequence by ensuring that the designs follow established rules of sequence construction. GenoCAD.org is a publicly available instance of GenoCAD that can be found at www.genocad.org. The source code is available from SourceForge to allow advanced users to install and customize GenoCAD for their unique needs.

This is a hands-on tutorial that will be broken down into two sessions. During the first session, the students will use GenoCAD's parts management system to build a library of parts that they will use to design several genetic constructs. The first session also includes an overview of GenoCAD's SBML-based simulation tool.

The second session focuses on more advanced features of the application. We will introduce the search engine to retrieve specific parts from large parts libraries. We will show how the design management tool allows users to quickly make several variants of a plasmid. Finally, we will show how to use the grammar editor to customize the design rules associated with a specific project. The tutorial material is published on figshare.org. Prospective students are encouraged to review the material prior to signing up for the tutorial.

Participants should bring their laptop as the tutorial will be based on a series of practical exercises.

CASyM workshop: Should systems medical training be integrated for basic and clinical researchers?

Mikael Benson, Mika Gustaffson, Marc Kirschner, Hans Westerhoff, Gerold Baier, Charles Auffray, David Harryson, Damjana Rozman

Systems medicine is a multi-disciplinary field, which will soon have a large impact on clinical research and practice. Despite this there are limited training opportunities for basic and clinical researchers, and few that integrate such training. The aim of this workshop is to present experiences from systems medical training and finally to discuss the need for integrated training. The final discussion will be very open and welcome contributions from the auditorium.

PROGRAM

14.00-14.40. Experiences from systems medical training and future implications. Hans Westerhoff 14.40-15.00. Facilitating the integration – An eLearning platform for Systems Medicine. Gerold Baier 15.00-15.15. Coffee break

15.15-16.00. Systems medicaltraining from basic, clinical and pathology perspectives. Charles Auffray, Mikael Benson, David Harryson, Damjana Rozman

16-16.30. Should systems medical training for basic and clinical researchers be integrated? If so how? Open discussion moderated by Mikael Benson and Damjana Rozman

AllBio workshop on Standardisation Operation Procedures (SOP)

Susanne Hollmann, Babette Regierer

and

The integration of data for modelling is a critical step where intelligent rules play an essential role for the success. As systems biology needs to integrate heterologous and complex data to build models, the need for data standards in the life sciences becomes an urgent topic. Therefore, systems biology could play a major role in the development of new and helpful standards for the production of high quality data. Systems biology could therefore be a driver for standardisation processes in the life sciences in general.

The systems biology community needs the close cooperation with data generation groups and the bioinformatics world to define a strategy how to generate the high quality data in the life sciences needed for model generation.

The workshop will address questions on standardization activities and processes in the life sciences with specific emphasis on systems biology needs. It also offers fundamental information about the creation of economically reasonable conditions for future industrial application.

Standard operating procedures (SOPs) for the generation and processing of data are highly important for data integration and model creation in particular in respect to because only the use of standards lead to

- high quality and comparable data, regardless of the sample origin and environment,
- for the use and application of results for industrial exploitation (e.g. in Synthetic biology).

The development of SOPs can also feedback and thus have impact to the creation of new standards.

During the workshop 'Standardizing Data and Metadata in Systems Biology' experts will provide an inside view on the processes around standardisation on the national (e.g. German) and international (CEN, ISO) level, followed by an overview on ongoing initiatives on standardisation (e.g. COMBINE, ISBE, AllBIO) in different life science areas. In a final discussion with the participants it is expected to define challenges and needs for standardisation activities in the systems biology and – if possible – also in the whole life science area. As a consequence, strategic considerations will be developed addressing key stakeholders on the European level. Thus, the systems biology community could benefit from the prominent role and be a driver in this area influencing the way how data are generated in the life sciences in general.

Tutorial: Modelling and Simulation of Quantitative Biological Models

Martin Golebiewski, Frank Bergmann, Akira Funahashi, Noriko Hiroi, Mike Hucka, Nicolas Le Novère, Pedro Mendes, Ion Moraru, Sven Sahle, Jacky Snoep, Dawie van Niekerk, Andreas Weidemann, Katy Wolstencroft

In this tutorial participants will learn setting-up quantitative computer models of biological networks using experimental kinetic data and simulating them in different systems biology platforms. Hands-on sessions, lectures and software demonstrations will be included providing attendees with the necessary skills to enable them to access experimental kinetics data from available resources, assembling computer models with these data and finally simulating the models within different tools.

Target audience:

Modellers and experimentalists with some basic experience in modelling and simulation of biological networks. Attendees are expected to bring their own computer.

The topics will include:

- Using experimental data for setting up quantitative models
- Parameter estimation, optimization and model fitting
- Simulation, analysis and visualization of biochemical models
- Integrated data management and model databases
- Community standards and formats for systems biology models

Covered tools, platforms, databases and standards:

BioModels database: http://www.ebi.ac.uk/biomodels-main/

CellDesigner: http://www.celldesigner.org/

COMBINE: http://co.mbine.org/ COPASI: http://www.copasi.org

JWS Online/OneStop: http://jjj.biochem.sun.ac.za/

SABIO-RK: http://sabio.h-its.org/

SBML: http://sbml.org

SYCAMORE: http://sycamore.eml.org SysMO-DB: http://www.sysmo-db.org/

Virtual Cell (VCell): http://www.nrcam.uchc.edu/ Virtual Liver SEEK: http://seek.virtual-liver.de/