

10:00 AM Rhythm Analysis in Dynamical Systems

Patrick Pett, Hanspeter Herzel Group, Charité and Humboldt University Berlin

Patrick will give a basic introduction into rhythmic systems of differential equations, bifurcation analysis and a clamping method developed in the lab. The tutorial would be practically oriented using numeric simulations in R such that specific mathematical background knowledge is not required. Participants can run simulations in R during the tutorial or just listen and have a look at the example files later.

11:30 AM Review: Computational Methods for Metabolite Identification

Dai-Hai Nguyen, Mamitsuka Lab, Kyoto University

Metabolomics involves studies of a great number of metabolites, which are small molecules present in biological systems. They play a lot of important functions such as energy transport, signaling, building block of cells and inhibition/ catalysis. Understanding biochemical characteristics of the metabolites is an essential and important part of metabolomics to enlarge the knowledge of biological systems. It is also the key to the development of many applications and areas such as biotechnology, biomedicine or pharmaceuticals. However, the identification of the metabolites remains a challenging task in metabolomics with a huge number of potentially interesting but unknown metabolites. The standard method for identifying metabolites is based on the mass spectrometry (MS) preceded by a separation technique. Over many decades, many techniques with different approaches have been proposed for MS-based metabolite identification task, which can be divided into four groups: mass spectra database, *in silico* fragmentation, fragmentation tree and machine learning. In this tutorial, Dai-Hai will survey currently available tools for metabolite identification with the focus on machine learning based approaches. He will also lead an intensive discussion on advanced machine learning methods, which can lead to further improvement on this task. Laptops are not necessary for this tutorial.

12:00 PM Lunch

12:30 PM Community Modeling/COMETS tutorial

Ilija Dukovski, PhD, Segrè Lab, Boston University

In this workshop Ilija will cover the basics of dynamic Flux Balance Modeling, as implemented in COMETS. (<http://comets.bu.edu>). After a short presentation on the theoretical background of the methodology, students will have the opportunity to have a hands-on experience of setting up and running several simulations of bacterial communities. The examples will include single species and co-culture communities, in homogeneous, as well as spatially structured environments. Please bring a laptop, if possible.

PLEASE RSVP TO CAROLINE

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