

# Abstract

The metabolism constitutes the universe of biochemical reactions taking place in a cell of an organism. These processes include the synthesis, transformation, and degradation of molecules for an organism to grow, to reproduce and to interact with its environment. A good way to capture the complexity of these processes is the representation as metabolic network, in which sets of molecules are transformed into products by a chemical reaction, and the products are being processed further. The underlying graph model allows a structural analysis of this network using established graphtheoretical algorithms on the one hand, and a visual representation by applying layout algorithms combined with information visualization techniques on the other.

In this thesis we will take a look at three different aspects of graph visualization within the context of biochemical systems: the representation and interactive exploration of static networks, the visual analysis of dynamic networks, and the comparison of two network graphs. We will demonstrate, how established infovis techniques can be combined with new algorithms and applied to specific problems in the area of metabolic network visualization.

We reconstruct the metabolic network covering the complete set of chemical reactions present in a generalized eucaryotic cell from real world data available from a popular metabolic pathway data base and present a suitable data structure. As the constructed network is very large, it is not feasible for the display as a whole. Instead, we introduce a technique to analyse this static network in a top-down approach starting with an overview and displaying detailed reaction networks on demand. This exploration method is also applied to compare metabolic networks in different species and from different resources. As for the analysis of dynamic networks, we present a framework to capture changes in the connectivity as well as changes in the attributes associated with the network's elements.