

Poster: Interactive Navigation in Interconnected Biochemical Pathways

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ABSTRACT

Approaches to investigate biological processes have been of strong interest in the last years and are in the focus of several research areas, especially Systems Biology. Biochemical networks are very important for such a comprehensive understanding of living beings. Drawings of these networks are often visually overloaded and do not scale. A common solution to deal with this complexity is to divide the complete network into a large set of single pathways that are hierarchically structured. In this poster paper, we present a solution of visualizing and navigating interconnected biochemical pathways.

Keywords: Network visualization, biochemical networks, navigation, glyphs.

Index Terms: I.3.6 [Computer Graphics]: Methodology and Techniques—Interaction Techniques; I.3.8 [Computer Graphics]: Applications; J.3 [Life and Medical Sciences]: Biology and Genetics

1 INTRODUCTION

The visualization of large and complex networks is still one of the most challenging tasks in graph drawing and information visualization [4]. Even if considerable work on graph visualization has been done in the literature and powerful tools exist, some fundamental problems are not sufficiently solved. For example, drawings of huge biochemical networks are often visually overloaded and do not scale. One traditional solution is a hierarchical structuring of the entire network if possible, i.e., the complete network is divided into many parts [3]. If these pathways are visualized, then additional navigation and exploration problems occur, because the user loses the overview on the entire network.

In this poster paper, we present a general approach of navigating between interconnected subgraphs and discuss it in context of biochemical networks, i.e., in a set of hierarchically structured pathways (groups and sub-groups of pathways). Our new visualization approach initially supports the researcher to get an overview of pathways, which are connected to the currently considered pathway via its nodes and edges. Based on this context information, our tool is able to intuitively guide the exploration and navigation process by using glyphs, brushing, and topological information of the involved pathways. To deal with real data, current networks and concrete problems, we decided to implement our approach as a plugin for the VANTED system [2].

Data Sets Here, we use the MetaCROP database [1] that summarizes diverse information about metabolic pathways in crop plants and can be directly accessed by VANTED. The pathways are placed in six groups consisting of 38 pathways in total. Thus, the MetaCROP hierarchy has two levels. In MetaCROP, metabolites are depicted as circular nodes; proteins (enzymes or transporters) are shown as rectangular nodes. We have also successfully tested our approach with the KEGG data set [3], but the mapping of KEGG hierarchies/groups is not completely implemented yet.

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2 NAVIGATION APPROACH

In a first step, we developed small *navigation glyphs*, which are embedded within the network nodes. They show the pathway link situation outgoing from a specific node, see Figure 1. The color coding of the “glyph petals” represents the pathway group (level 1 in the hierarchy), while their size/length shows if there is a link (to the same node in another pathway) or not. Thus, our navigation glyphs provide a good and simple overview about the relationships to connected pathway groups outgoing from a single node. By a right click on a node, the system displays a context menu with a list of links to all connected pathways. Then, a new pathway window is activated after a click on a specific link.

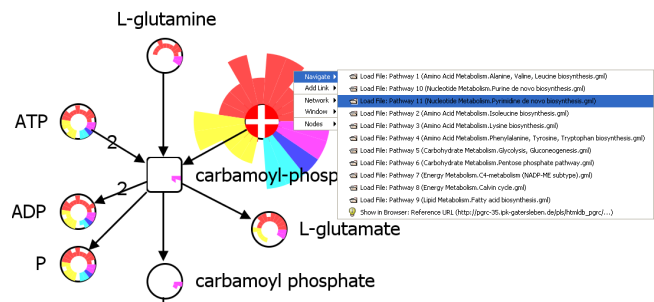


Figure 1: Embedding of our *navigation glyphs* into some nodes of a (focus) pathway. The glyph of the currently selected node is highlighted and magnified by the system. With a right mouse-click the user is able to open a context menu with a link list from which he/she can jump to connected (target) pathways.

Our main idea is to extend the navigation glyphs by (1) providing an overview of all connected pathways of the current focus pathway, (2) showing statistical information about the focus pathway’s link distribution, and (3) facilitating the navigation from nodes in the focus pathway to different target pathways. For this, we introduce new visualization and brushing techniques coupled with seamless interaction of various parts of the system. That makes the navigation of different pathways easier and yields a more intuitive exploration experience. We also introduced a possibility to compare the number of total references to all connected pathways.

Navigation Window The approach consists of laying out mini-sized images of pathway drawings, called *graph icons*, around the main view that contains the currently considered focus pathway, see Figure 2. Both together form the *navigation window* of our VANTED plugin. The graph icons are used to navigate to a specific pathway by mouse clicks, which would load the target pathway into the navigation window. Each graph icon has a background color that is brushed accordingly to the color coding of the navigation glyphs within the pathway nodes, thus making it easy to identify different pathway groups of the MetaCROP data set. The user is able to recognize the pathways connected to the nodes of the focus pathway based on their graph topology, additionally supported by the aforementioned color coding. For precise information about the pathways, tooltips show the names of the pathway and of the pathway group. They appear based on a mouse-over event of a specific graph icon. Note that the position of the graph icons corresponds to the position of the petals within the small *navigation glyphs*.

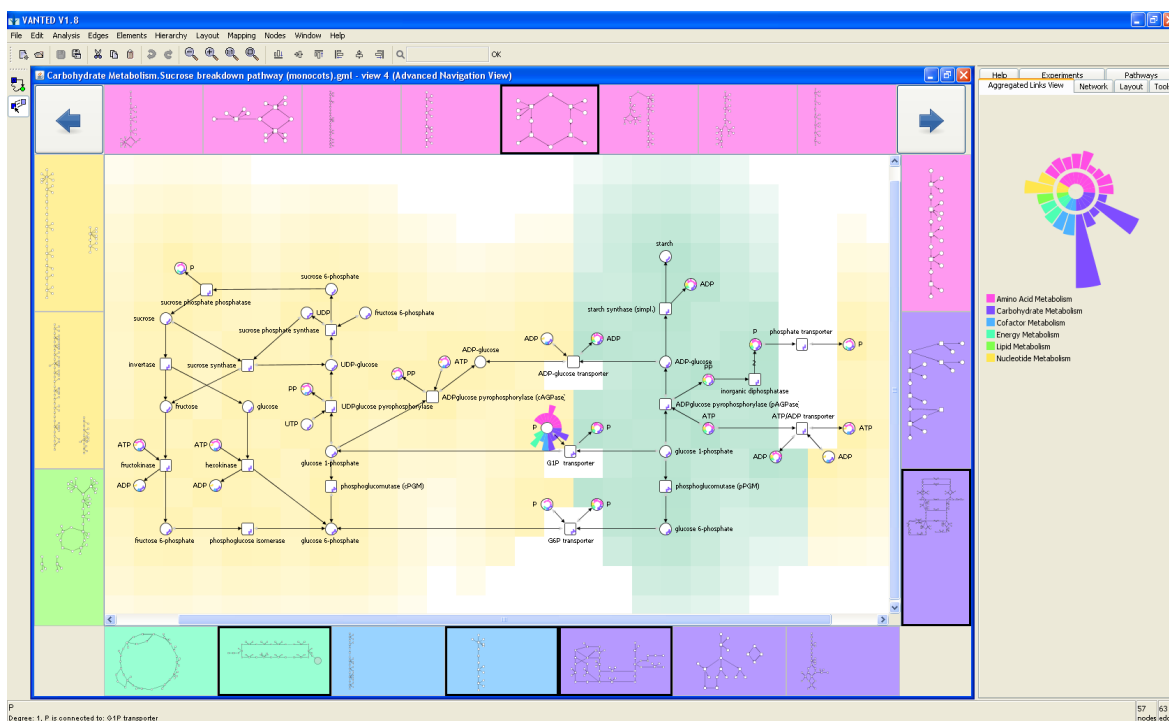


Figure 2: Overview of the new VANTED plugin with the *navigation window* on the left and the *aggregated links view* on the right. The background coloring of the focus pathway shown in the navigation window represents different cell compartments. One node is selected and its navigation glyph was magnified by the system. The glyph petals are directed to the surrounding graph icons. Links to other pathways are double-coded by the longer petals as well as by the highlighted graph icons (via black frames).

By the graph icons, it is now possible to navigate through all related pathways using one window, while providing a good overview of all pathway links. Users can easily access all pathways linked from an interesting node through a mouse-over, which will highlight the corresponding graph icon. This feature allows users to quickly navigate and/or to gain insight into the connectivity of desired pathway components. Additionally, the user might use *back* and *forward buttons* to facilitate the navigation. They can be found on the left and right upper corner of the navigation window. Based on a mouse-over action, these buttons will also highlight the graph icon, which represents the previously visited pathway.

Aggregated Links View The graph icons provide an overview of all pathways linked to the current focus pathway, but they cannot show the frequency a particular target pathway is being referenced from the nodes of the focus pathway. Thus, we added a separate interactive diagram placed at the right upper corner in a tab, called *aggregated links view*, to present this data (the other tabs are provided by VANTED). Figure 2 shows this diagram on the right hand side. As it resembles the navigation glyphs and is able to guide the user like a traditional compass rose metaphor, we called it *link rose*. In contrast to the navigation glyphs that represent the links of a particular pathway node, it displays the number of *all* links to other connected pathways in context of the current focus pathway. Thus, it enables users to compare all outgoing pathway links and to show which pathways are strongly connected to the focus pathway.

Mouse-over actions on a rose petal will show a tooltip with additional information of the corresponding pathway. Following the idea of several coordinated views [5], a click on a rose petal initiates that all graph nodes referencing to the selected pathway are also highlighted in the navigation window.

3 CONCLUSIONS

We presented a novel solution to guide the navigation and exploration process of interconnected pathway visualization and dis-

cussed it in context of biochemical networks. Our visualization approach supports the analyst to get an overview to connected pathways if he/she is working within the currently focused pathway.

User Feedback We discussed our plugin with four domain experts from the IPK Gatersleben. These experts (biologists and biochemists) are used to work with metabolic pathways and are familiar with pathway databases such as KEGG and MetaCrop, as well as with the VANTED system. After a short introduction to the idea of the navigation method, we asked the experts to work with the plugin, to investigate the metabolic pathways stored in the MetaCrop system, and to provide feedback. The experts described the navigation through the different pathways as intuitive and very helpful. The used colors and the size of the glyphs were considered appropriate, the speed of navigation (e.g., replacement of one pathway by the next one) as fast enough. In particular, the interaction between the *link rose* and the pathway was considered as useful in order to select nodes occurring in another pathway.

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