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INTERACTIVE VISUALIZATION OF METABOLIC PATHWAYS

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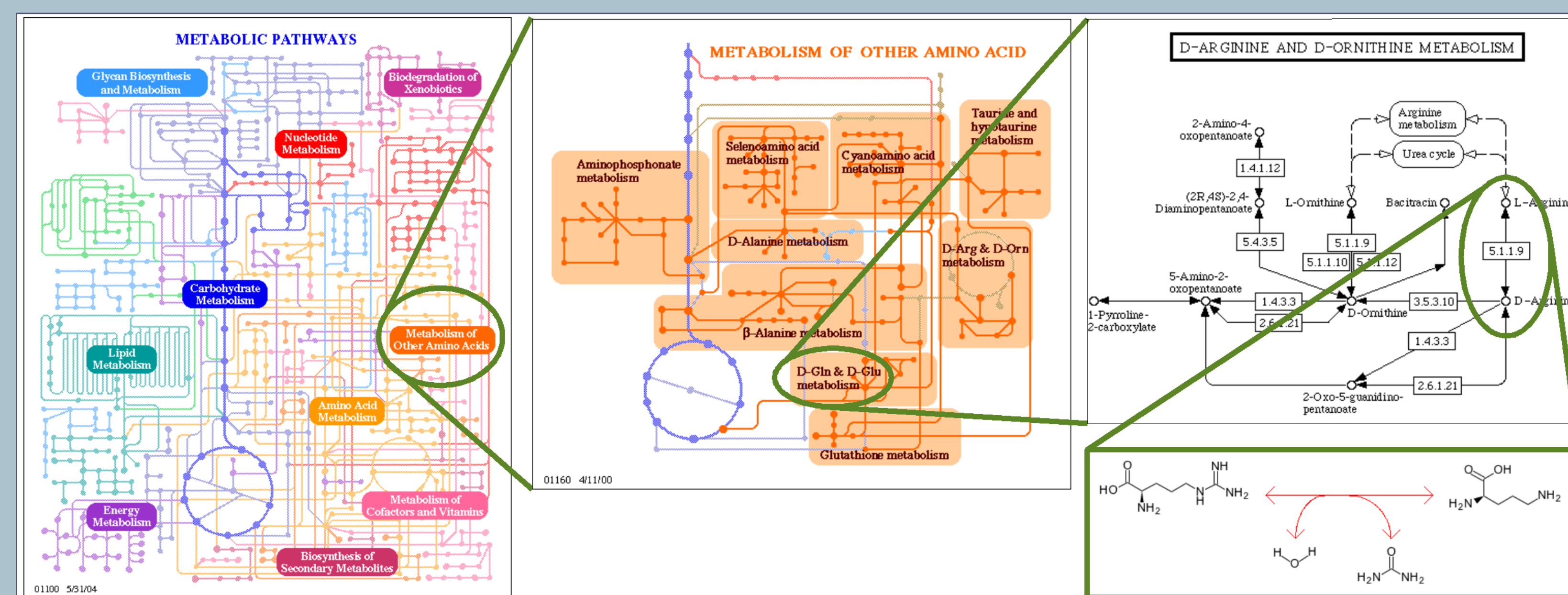
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ABSTRACT

This work enriches the visualization of **complex graphs** from the **biomedical domain** called metabolic pathways by means of interactive **linked views in 2D and 3D**. Due to the high degree of complexity of pathways biologists are restrained by currently available systems in the process of **hypothesis generation and validation**. We propose an interactive visual data- mining process that is supported by the integration of methods such as **details-on-demand** and **focus and context.**

INTRODUCTION TO METABOLIC PATHWAYS

Metabolic pathways represent cellular functions and are therefore important for the daily work of biologists and pathologists. Metabolic pathways are directed non-planar graphs consisting of two types of nodes namely chemical substances and enzymes. Inside regular metabolic pathways enzymes are linked to compounds and may have multiple fan-in and multiple fan-out. Enzymes and compounds can appear several times in different sub-groups as well as in one sub-graph.
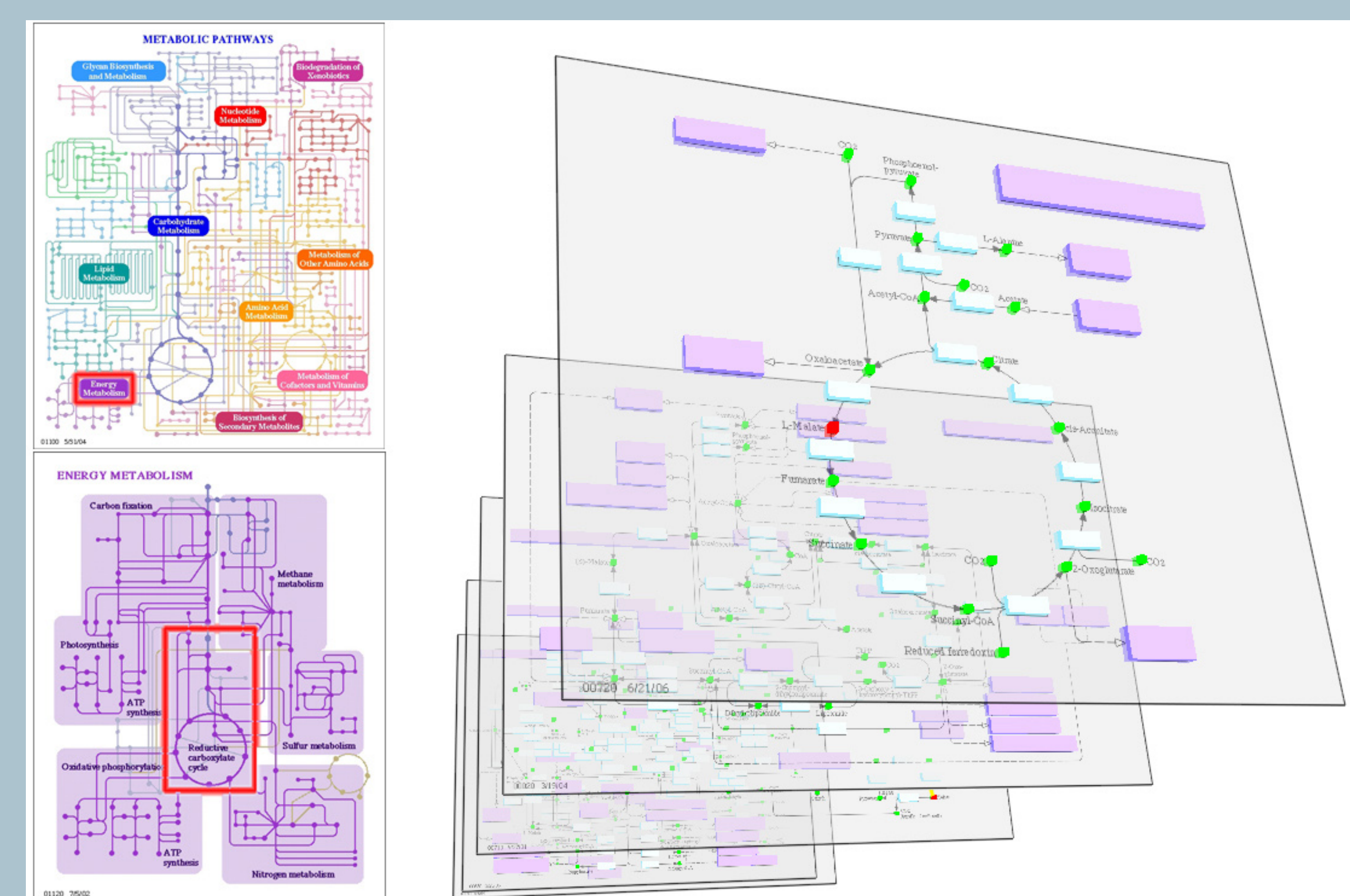
Metabolic pathways can be grouped hierarchically in 4 levels. The first 3 levels represent different biomolecular properties while the fourth, bottom level, consists of chemical reactions only. Since pathways describe biological properties, one pathway can be linked or embedded inside another pathway. This is a side effect of flattening the non-planar graph.

Our contribution is not a new layout algorithm for non-planar graphs, but a new way to interact with huge graphs using several linked views. We rely on existing layout algorithms and on hand-crafted graphs as used in the KEGG database. The KEGG layout is used as a background texture where the nodes are superimposed onto. This approach does not require to layout the edges while allowing interactive manipulation based on the familiar KEGG representation.
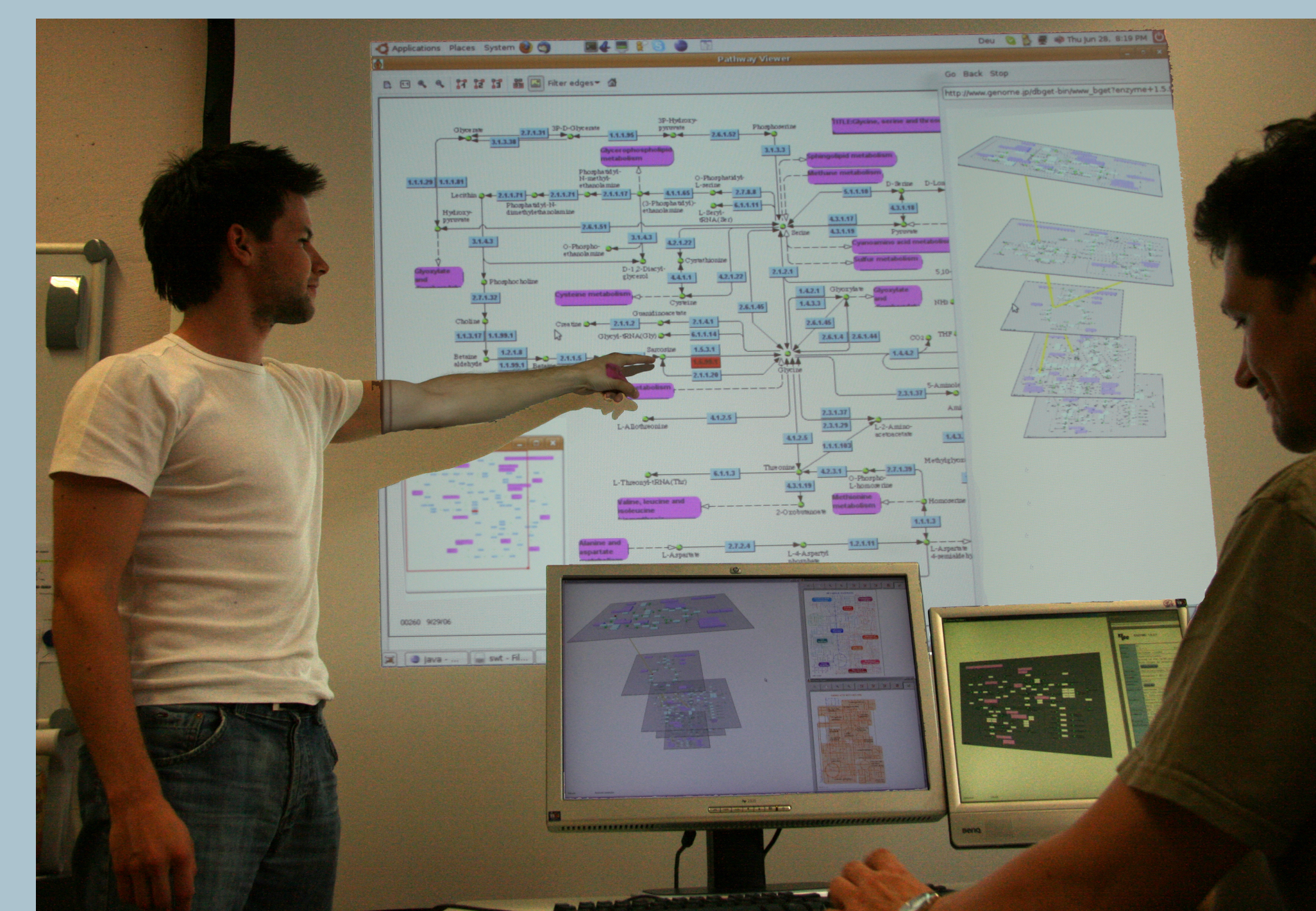
MULTIPLE VIEWS USING 2D AND 3D

We propose the usage of multiple views showing different portions and scales of the metabolic graphs. The graphs are also available in multiple layout variants, essentially semantic level of detail. Linked views allow showing all instances simultaneously. We address this issue by visually linking multiple nodes in 2.5D views. Once the user starts switching pathways it is difficult to keep it in context. Adding two more views of the root level and the intermediate level of the hierarchy and linking them to the current selected pathway helps the user to achieve that. The current pathway is highlighted in the two other views.

We also propose to show several pathways as planes in 3D to be able to present and interact with them concurrently. This also enables us to depict multiple occurrences of one node denoted as enzyme or compound in several pathways. The pathways can either be selected by the user due to special interests or switched and loaded dynamically depending on one enzyme or one compound.

MULTI USER SETUP

Our approach targets either a multiple desktop setup or a multi-user setup including a projector for collaborative data analysis. This setup consists of a projection wall and 2 LCD screens. Multiple views enable the user to trace several links of an enzyme or compound visually instead of opening many websites at a time and keeping the threads together in the mind of the user. Our proposed 3D representation in combination with the traditional 2D pathway and the web browser enables the user to find hidden properties of the complex graphs.

INTERACTION WITH MULTIPLE VIEWS

The 2.5D view shows several pathways containing the same enzyme. Identical nodes in dependent pathways are interactively highlighted and connected to the selected one among the layers.

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GeneView is a joint research project of Graz University of Technology and Medical University of Graz