

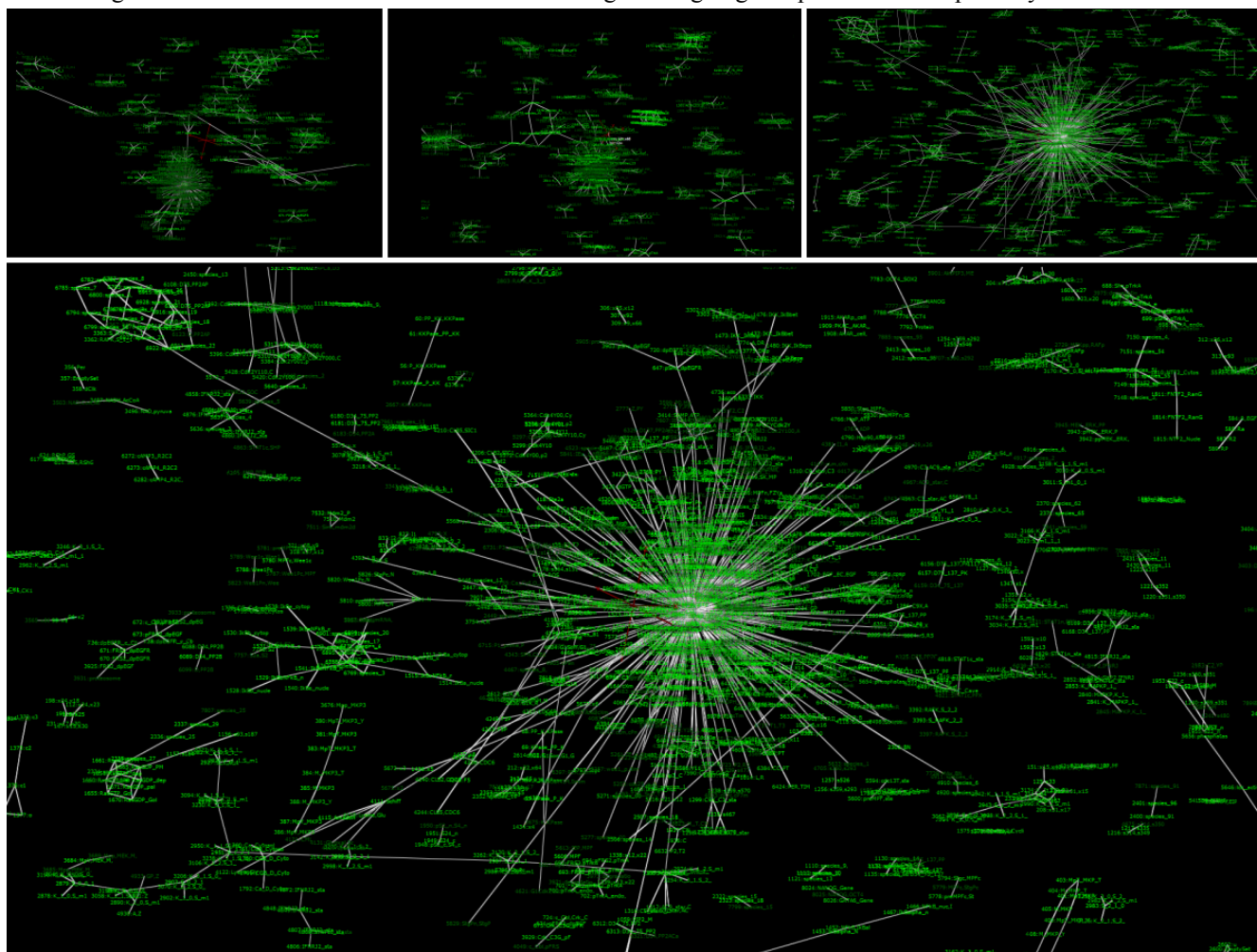
Editing and Aligning Complex Molecular Pathways Using 3D Models

B. Yankama¹, R. Umeton^{1,2}, S. Ayyadurai¹, and C. F. Dewey¹

¹Massachusetts Institute of Technology, Cambridge, MA, ²University of Calabria, Rende, CS, Italy

Cytosolve[1], allows multiple complex biological models created by different users to be combined in a manner that identifies common species and reactions. Unfortunately, as the number of models increases, the incidence of duplicate pathways also increases to the point where interpreting the text description of the overlaps is nearly impossible. This paper describes a graphical alignment tool for interpreting multiple pathways that interact with one another. We have developed a 3D graph modeler [Fig. 1] and interface to spatially visualize the reaction-relationships between duplicate species groups in different models identified by our parsing engine OREMP[2]. Each species-group involved in a reaction represents a node in the graph, while the reactions between nodes are represented as edges. Reaction-edges belonging to the same model are proximal. The alignment system was tested using 234 curated models from BioModels.net[3], which yielded 4830 nodes with 500 potentially duplicated reaction paths. We found our graphical/spatial interface to be extremely useful in gaining physical insight into the interactions. This visualization was implemented in Python and OpenGL using the vpython library. Clustering in space is K-dimensional in the number of each node's reaction edges, and overall positional layout is an N-body simulation, where nodes represent point-charges, edges are springs, and the Model to which each reaction-species-group belongs is a hidden attractor. This program will be open for public use on <http://cytosolve.mit.edu> website.

Figure 1. Screen-shot of the 3D interface for editing and aligning complex molecular pathways



[1] Ayyadurai, S. and Dewey, C.F. Jr. (2010) Cellular and Biological Engineering (In review).

[2] Umeton, R., et Al. (2010) Ontology Repositories and Editors for the Semantic Web (In press).

[3] Le Novere, N., et Al. (2006) Nucleic Acids Research.