BioReact: Visualization of Systems Biology Reaction Network

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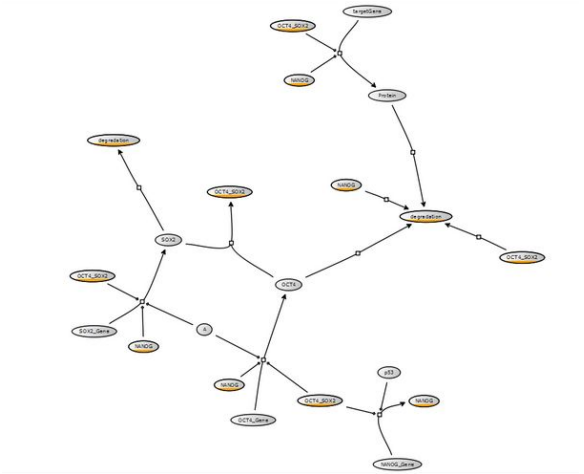
Introduction

- What is a Systems Biology Reaction Network?
  - A visual representation of cause-effect relationships between biological entities
  - The relationships form a large system, resembling a directed graph

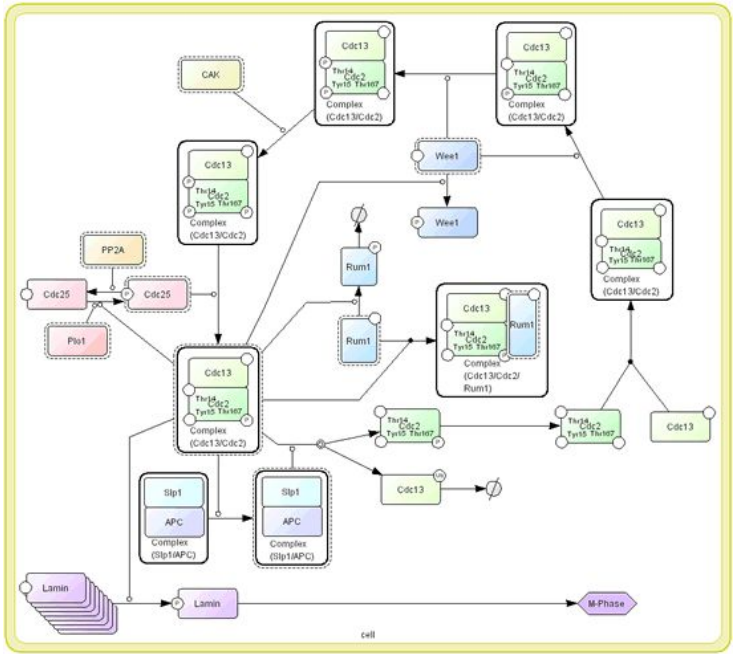


Problem

- Networks are very large, users do not know where to find datapoint of interest
- Nodes and links are cluttered, cause cognitive burden
- Related data are not close together, may take too much effort to find closely related data

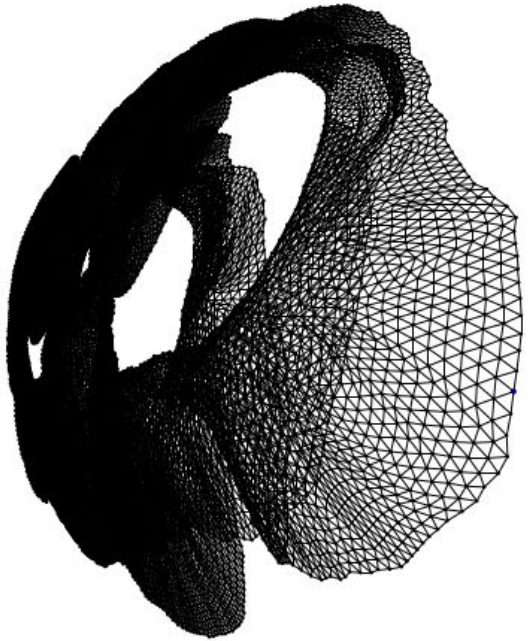
Related Work: CellDesigner (Brute Force)

- Explicitly specify (x,y) coordinates of each node and link



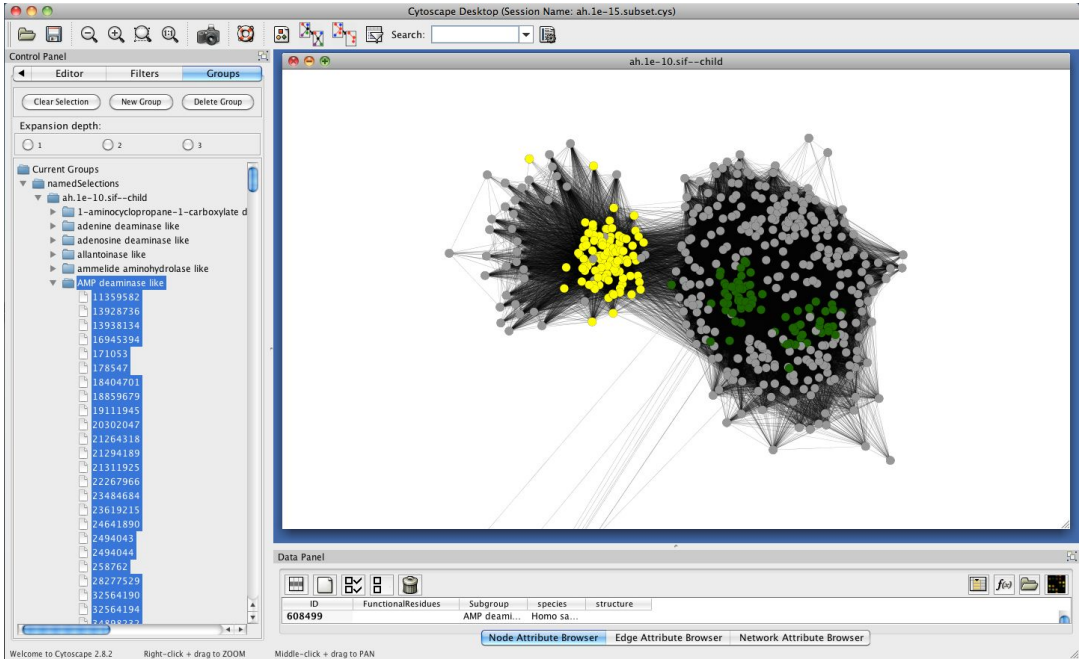
Related Work: Topological Fisheye Views

- Reduces clutter, but is not tailored for datapoint query or identification



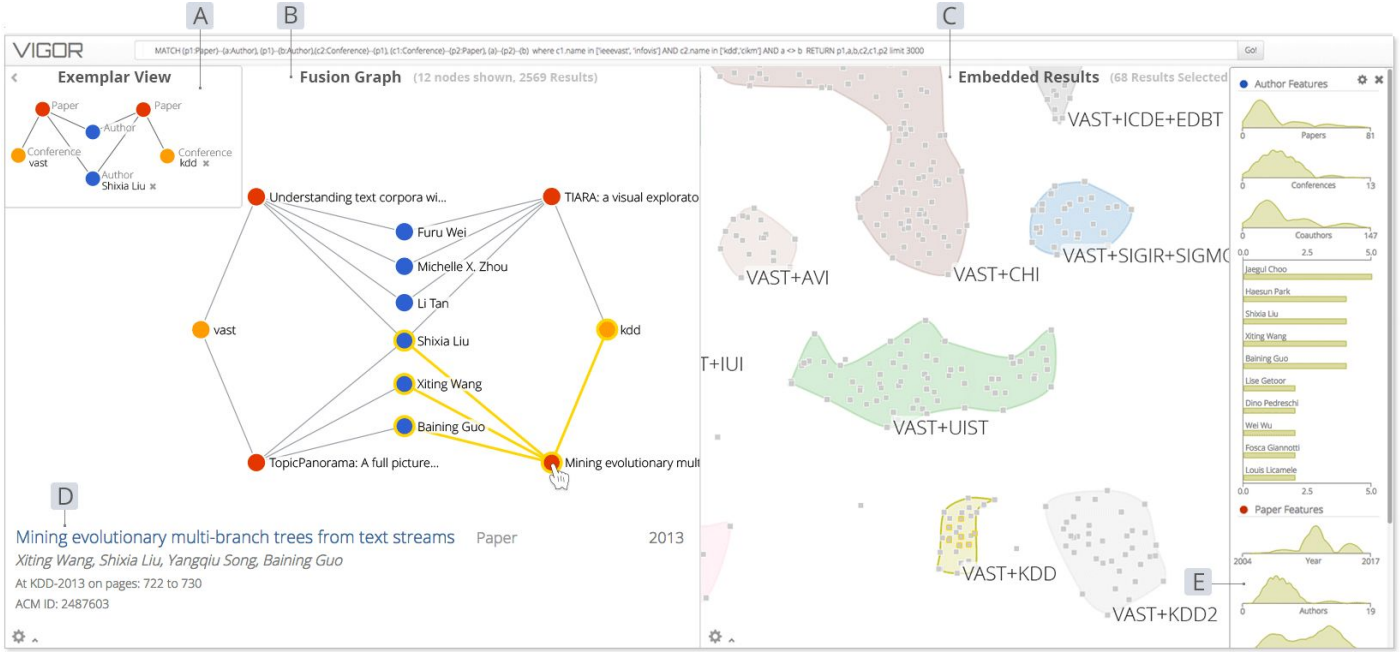
Related Work: Cytoscape

- For experts use only, too difficult to use for new users



Related Work: VIGOR

- Effective graph query, multiple coordinated views, filtering, and result summarization



Data Abstraction

- There are ~40000 nodes and ~100000 links in the complete network, distributed across ~600 models (static XML files)
- There are 2 categories of nodes, Species node and Reaction node.
  - The nodes are always connected alternately, i.e. Species and Reactions connect alternately forming a bipartite graph.
- Each node has additional categorical attributes:
  - id, name
- Each link has additional attributes:
  - source, target (categorical), value (quantitative)

What: Derived

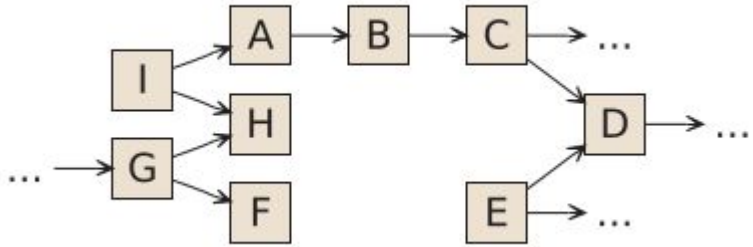
- Additional statistics were computed, such as:
  - How many times does a Species.name appear in the network?
  - How many times does a Species.id appear in the network?

Task Abstraction

- Present the network as node-link diagram to the user
- Allow user to **query** for a specific node by its name
- Allow user to **browse**, **locate**, and **explore** parts of the network
- Layout of the node-link diagram needs to clear enough to show **topology** of the network as well as **paths**

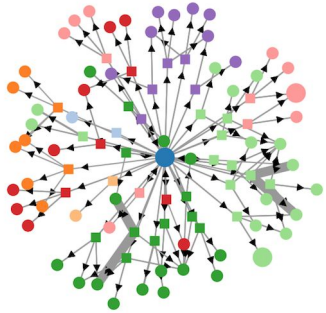
Applying Technique: IPSEP-COLA

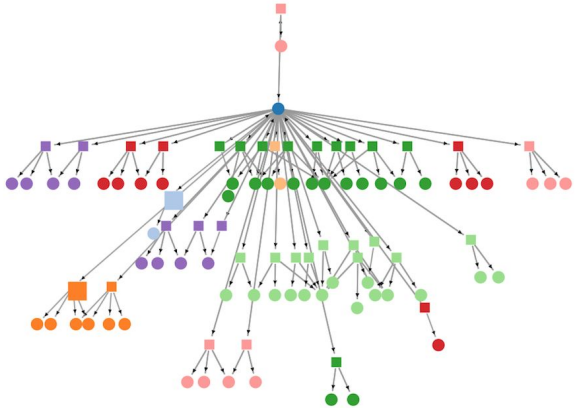
- Since the node-link diagram is directed, would be easier to preserve the flow direction of the links.
- Nodes are separated into different layers, constrained by avoiding overlaps between nodes and links

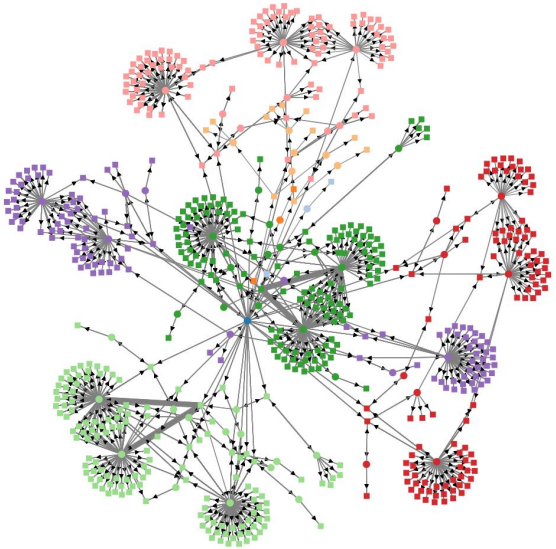


Our Network Structure

- Force Directed Layout
- Downward Layout (IPSEP-COLA)







Demo

How: Encode

- Species and Reactions: Nodes, circle and rectangle respectively.
- Links: Lines with arrow to denote the direction.
- Group: Color and Saturation.
- Value: Stroke Width of the Link.
- Specific Information: Text label triggered by clicking .
- Derived statistics: Bar chart

How: Reduce

- Query

  -By Species Name, Level, Direction

- Reduce

  -Provide multiple options to filter the searching result.

  -Reduce the complexity of the network.

- Dynamic Aggregation

How: Manipulate

- Navigate

  -scroll, drag to dynamically change the view.

- Select:

  -click the nodes in the network to get specific information.

  -click the node to make it bigger. Recover by clicking the blank area.

  -click two nodes to show path.

How: Facet

- Linked Highlighting

  -click the button on the sidebar to make the corresponding node bigger. Color to mark the button just clicked.

  -link the ordinal bar chart to the items in the search result.

Result

- A user-friendly interface.
- Two network alternatives.
- For Learner: Provide a more direct way to browse the database. Efficient for developing the knowledge topology.
- For Researcher: Cut off the tedious procedure to look up the species and reactions required in their project.
- For Administrator: Check the incomplete data or error.

Future Work and Limitation

- Optimization the user interaction by feedback. Provide a standard reaction diagram for each reaction node.
- From Vis to Data: Implement an interface to modify the database directly from the front-end.
- Traverse into more nodes in single model view.
- Integrate to a system to allow synchronized update.