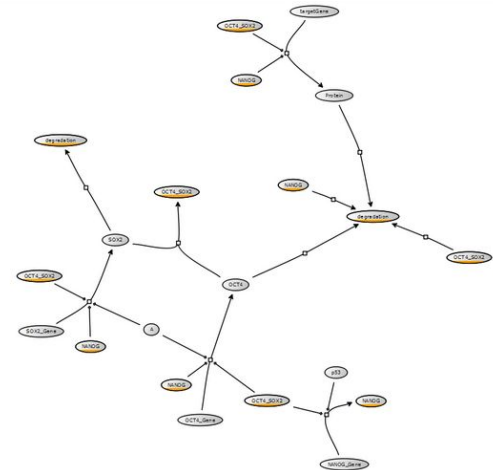


# BioReact: Visualization of Systems Biology Reaction Network

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2017.12.12

# 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



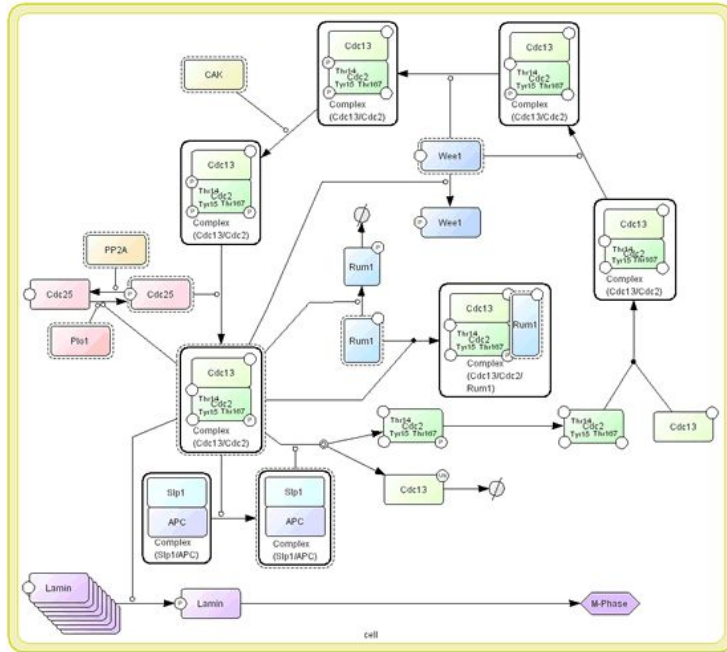
# Problem



- 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)

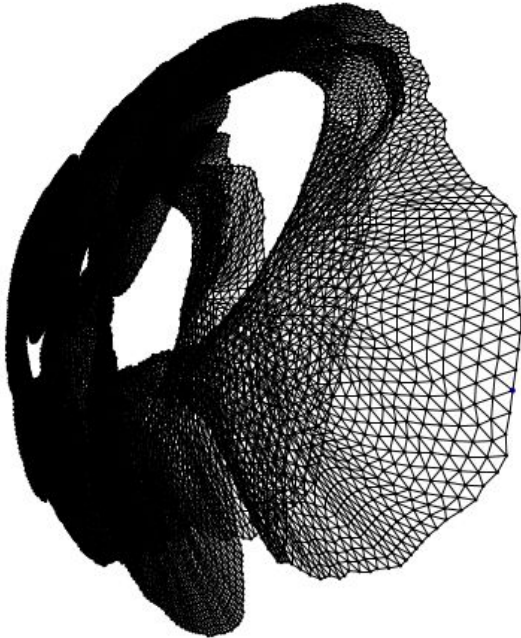
- Explicitly specify (x,y) coordinates of each node and link



# Related Work: Topological Fisheye

## Views

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



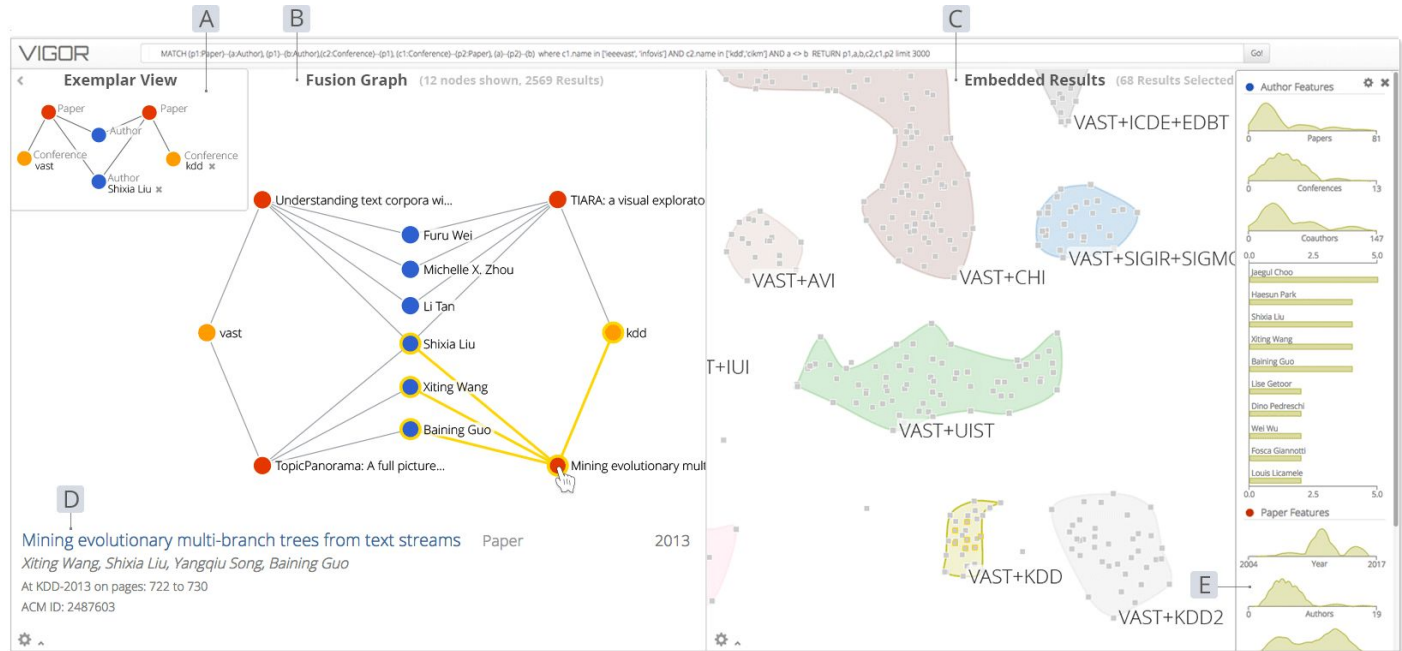
# Related Work: Cytoscape

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

The screenshot displays the Cytoscape Desktop application window. The title bar reads "Cytoscape Desktop (Session Name: ah.1e-15.subset.cys)". The main window shows a network graph with nodes and edges. A cluster of nodes is highlighted in yellow, and another cluster is highlighted in green. The interface includes a "Control Panel" on the left with tabs for "Editor", "Filters", and "Groups". The "Groups" tab is active, showing a tree view of "Current Groups" with "ah.1e-10.sif--child" selected. Below the tree, a list of node IDs is visible, including 11359582, 13929736, 13838134, 16945394, 171053, 178547, 18404701, 18859679, 19111945, 20302047, 21264316, 21294159, 21311925, 22267966, 23484684, 23619215, 24641890, 2494043, 2494044, 258762, 28277529, 32564100, 32564194, and 32603323. The "Data Panel" at the bottom shows a table with columns for "ID", "FunctionalResidues", "Subgroup", "species", and "structure". The selected node ID is 608499, with "AMP deami..." in the "Subgroup" column and "Homo sa..." in the "species" column. The "Node Attribute Browser" is active at the bottom.

# Related Work: VIGOR

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



# Data Abstraction

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- 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?

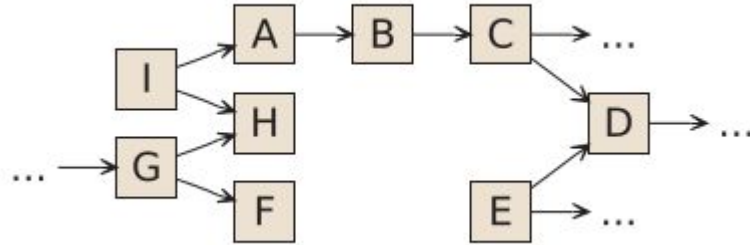
# Task Abstraction

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- 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 be clear enough to show **topology** of the network as well as **paths**

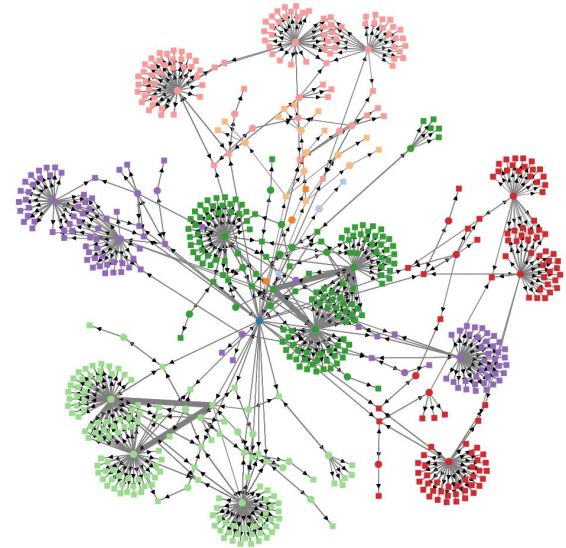
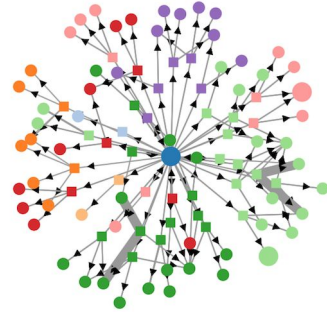
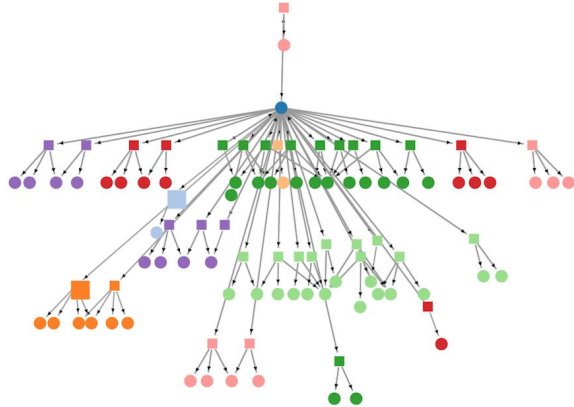
# Applying Technique: IPSEP-COLA

- 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

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- 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.