Visualizing Biomolecular Data
with the Caleydo Framework

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Graz University of Technology, Austria

CALEYDO

TU Graz

My Background: Austria

Our Institute

Institute for Computer Graphics and Vision
- Staff of about 80 people
- 4 Professors, 16 Post-Docs, 50 PhD students

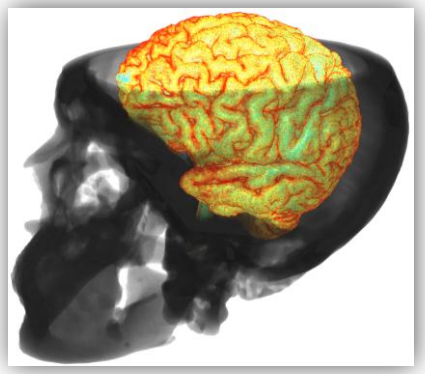
Computer Vision Group:
- Prof. Horst Bischof

Computer Graphics Group:
- Prof. Dieter Schmalstieg

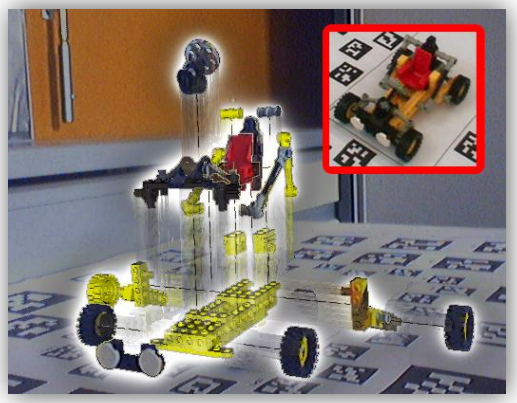
Research Areas

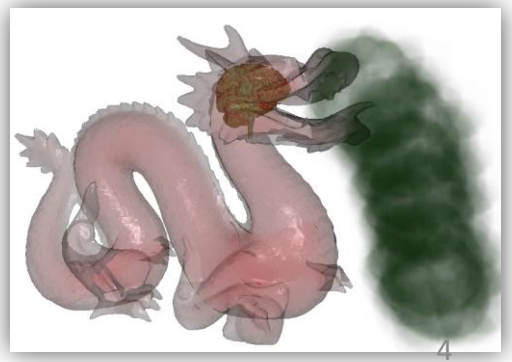
Augmented Reality

Multi-Display Environments



Volume Rendering / Medical Visualization





CALEYDO

Information Visualization and Visual Analytics

That’s what I’m talking about today!

InfoVis Research Topics

1. Visualization for biomolecular data
2. Connecting heterogeneous data sets

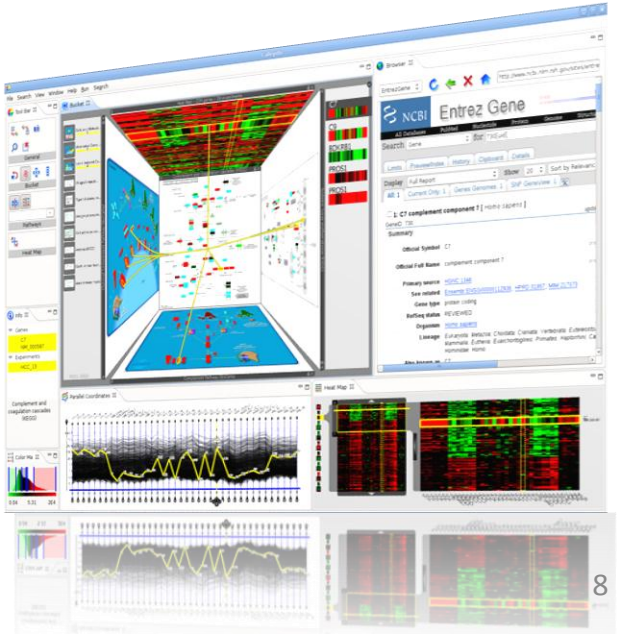
Find new visualization techniques and develop software that helps to understand the growing amounts of data in the life sciences

THE  PROJECT

What is Caleydo?

Visualization software developed with two goals:

1. Platform for creating novel visualization techniques
2. Tool that should actually help biologists



Features

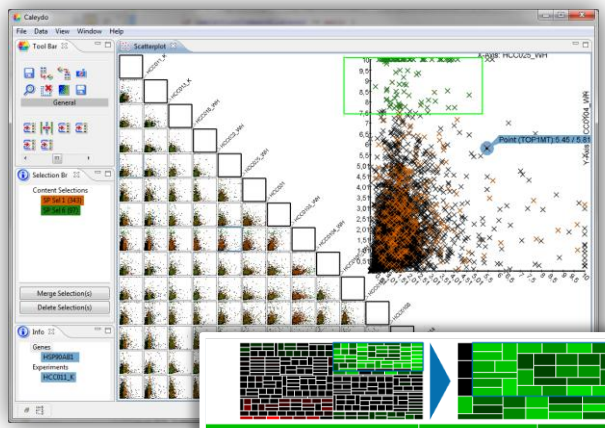
Various visualization techniques for tabular data and pathways

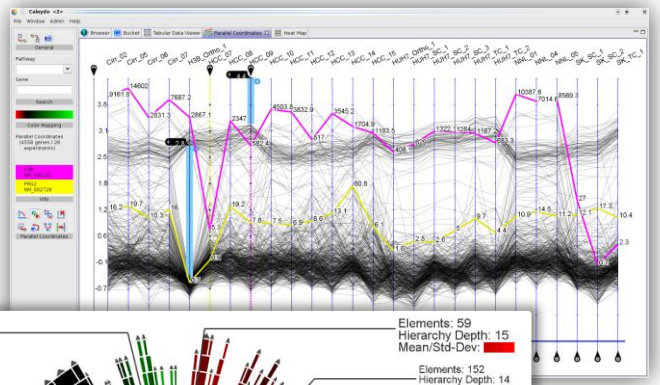
Runs on Windows and Linux (Mac yet to come)

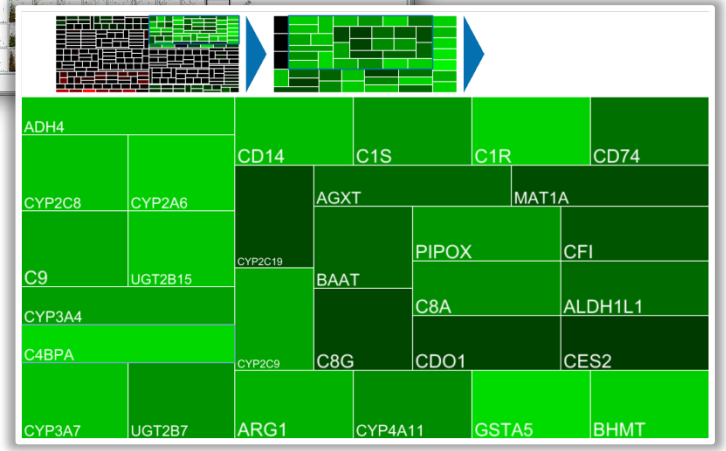
Analytical features:

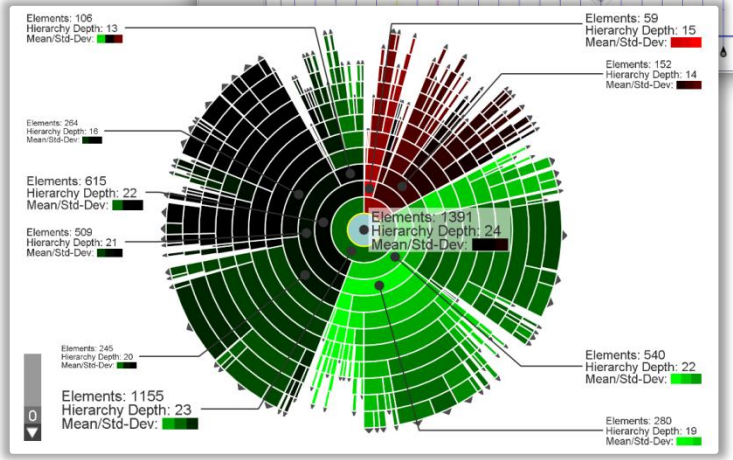
- R and WEKA interfaces
- Native clustering
- Fold Change, T-Tests, Variance Filters

Numerous Techniques









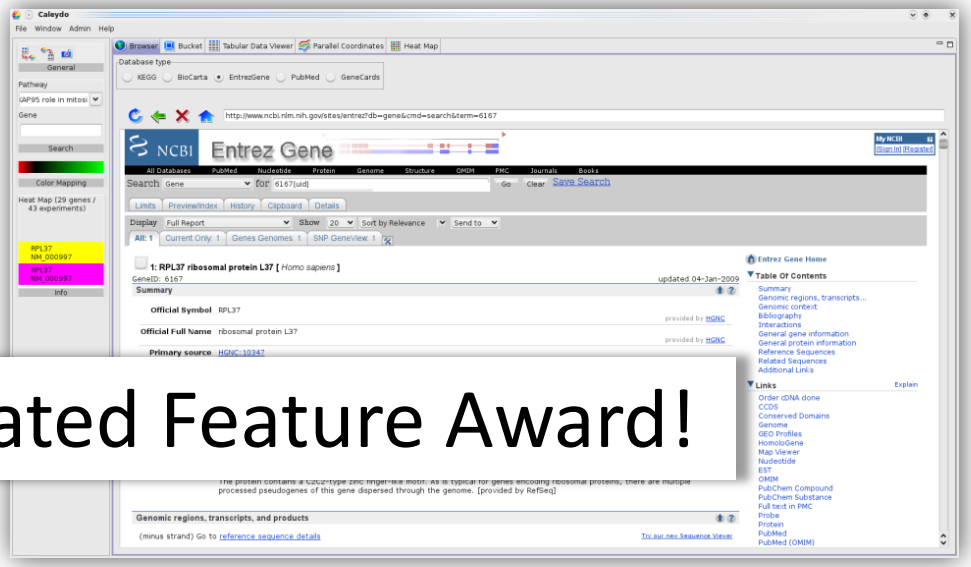
Linked Browser

Connected to major medical web databases

PubMed, Entrez,

KEGG, BioCarta,

GeneCards…



Most Appreciated Feature Award!

CALEYDO

VISUALIZATION FOR BIOMOLECULAR DATA

Research Topic 1

CALEYDO

Heat Maps

Common representation

Color coded magnitude of value

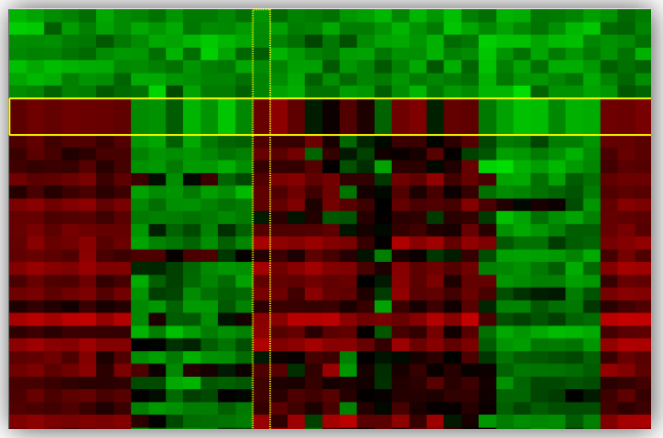
Filtering and clustering used

Problem:

do not scale well

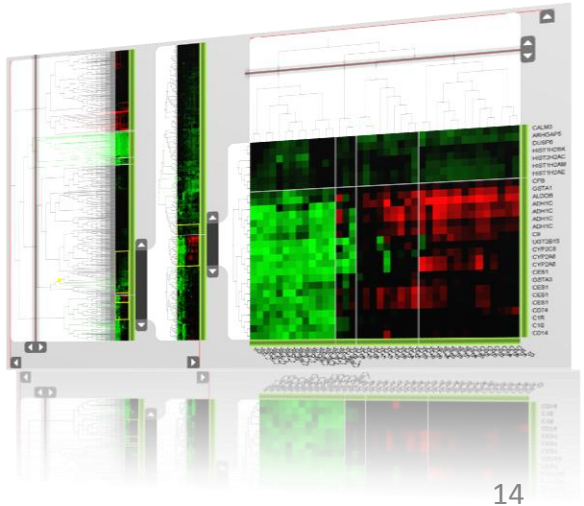
Solution:

hierarchical approach



[Lex, PacificVis 2010]

HIERARCHICAL HEAT MAP




Tool Bar
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Heat Map
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Browser
Entrez
NCBI
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Search
Gene
for
Limits
Preview/Index
History
Clipboard
Details
Display
Full Report
Show
Sort by
1: ADH6 alcohol dehydrogenase 6 (class V) [Homo sapiens]
GeneID: 130
Summary
The heat map uses three levels of detail to visualize a focus and its context.

Works well, but…

Tables often have homogeneous subgroups of dimensions

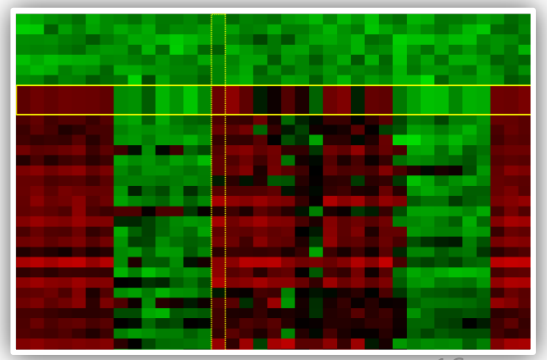
e.g., replicates, time-series, genotypes

Common task for multidimensional data:

Compare those groups

Traditional approach:

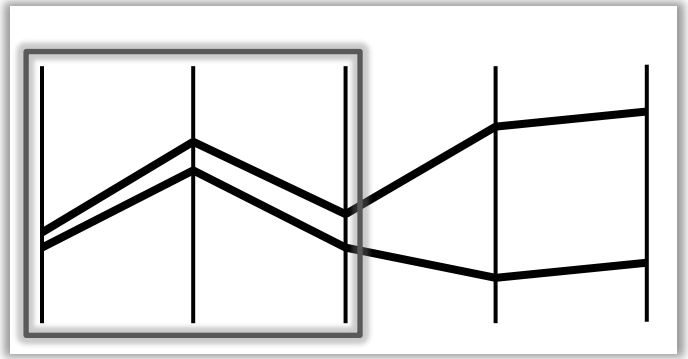
Filter, cluster all,
visualize with Heat Maps!



Clustering Inhomogeneous Data

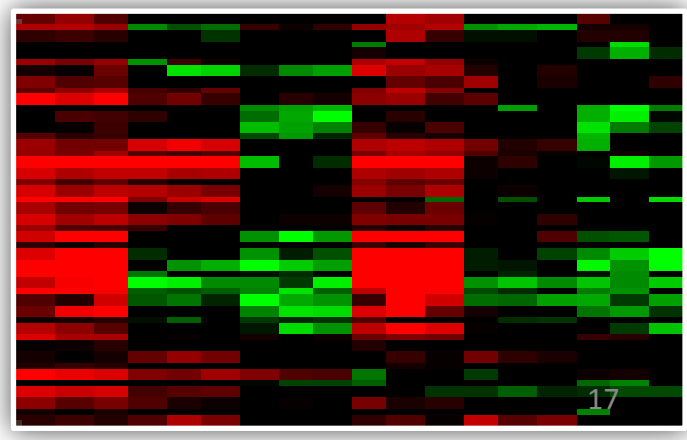
The Problem:

Clustering all dimensions at once obscures relations in homogeneous groups



The Solution:

Divide & Conquer!

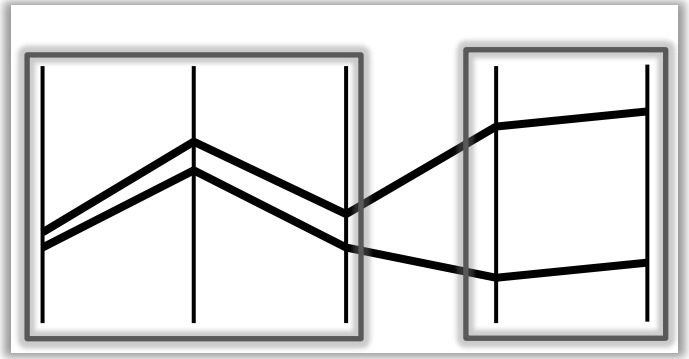


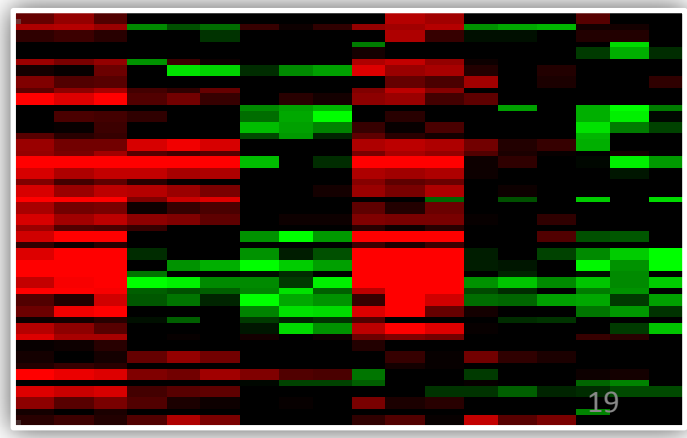
[Lex, InfoVis 2010]

MATCHMAKER

Clustering Inhomogeneous Data

Let's treat the groups separately!





Related Problem: Comparing Clustering Algorithms

Each run is one homogeneous group

Choice of algorithm, parameters and distance measures are important

No good quality metrics for clustering algorithms

- Visual assessment is best solution

The Process

1,1	1,2	1,3	1,4	1,5	1,6	1,7
2,1	2,2	2,3	2,4	2,5	2,6	2,7
3,1	3,2	3,3	3,4	3,5	3,6	3,7
4,1	4,2	4,3	4,4	4,5	4,6	4,7
5,1	5,2	5,3	5,4	5,5	5,6	5,7
6,1	6,2	6,3	6,4	6,5	6,6	6,7

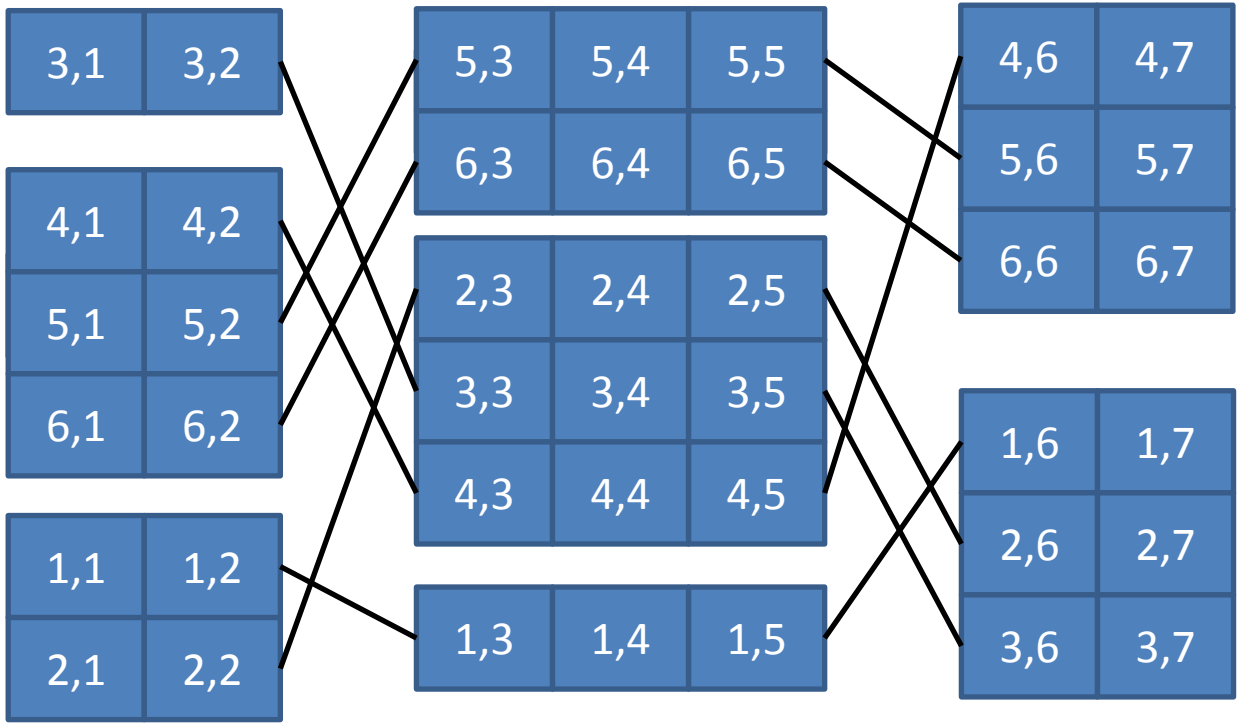
The Process

1,1	1,2
2,1	2,2
3,1	3,2
4,1	4,2
5,1	5,2
6,1	6,2

1,3	1,4	1,5
2,3	2,4	2,5
3,3	3,4	3,5
4,3	4,4	4,5
5,3	5,4	5,5
6,3	6,4	6,5

1,6	1,7
2,6	2,7
3,6	3,7
4,6	4,7
5,6	5,7
6,6	6,7

The Process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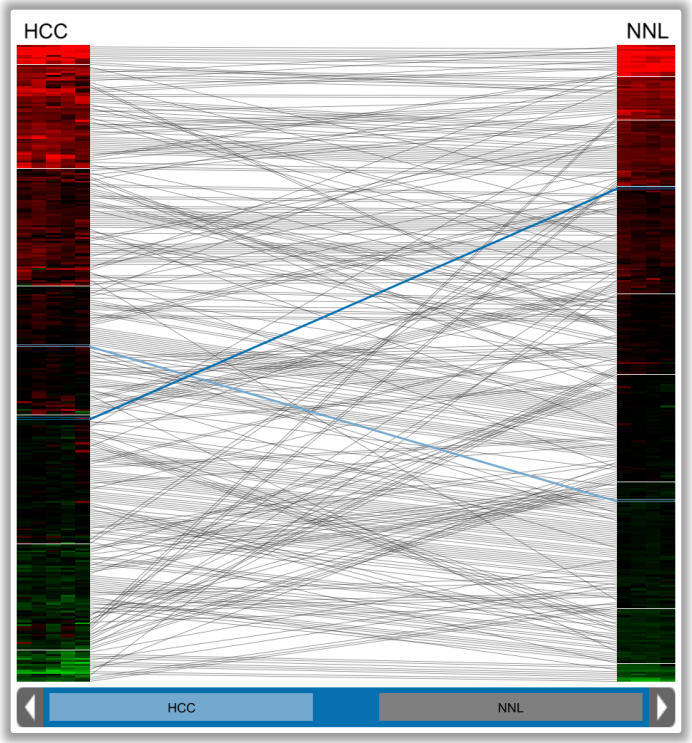
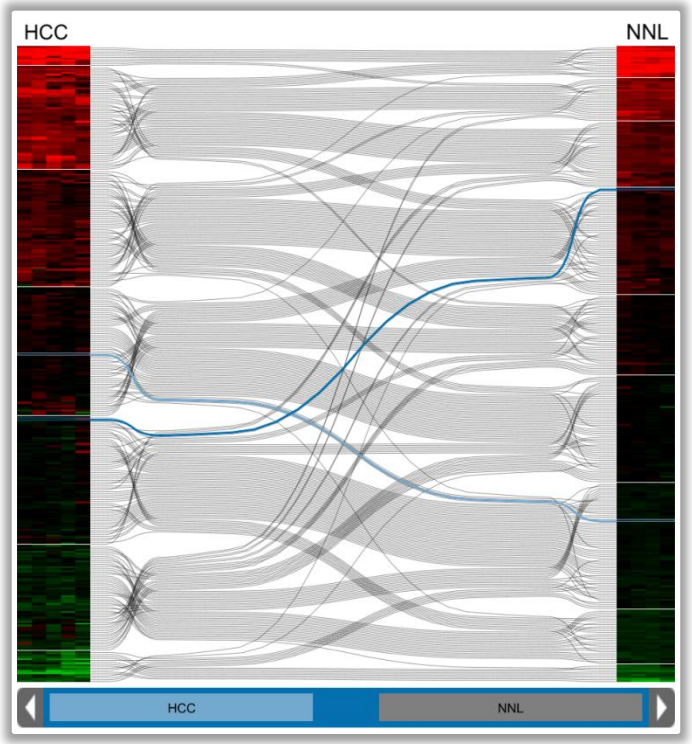
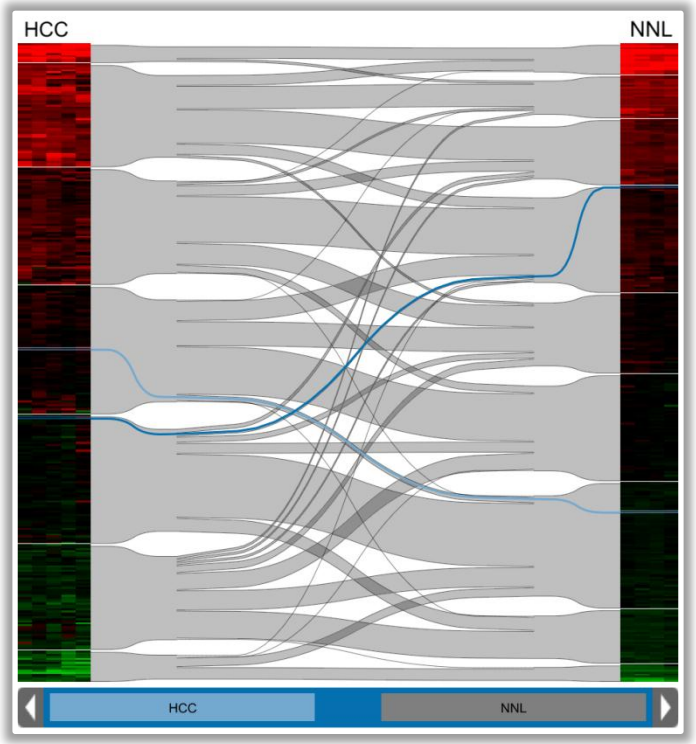
Immediate Result

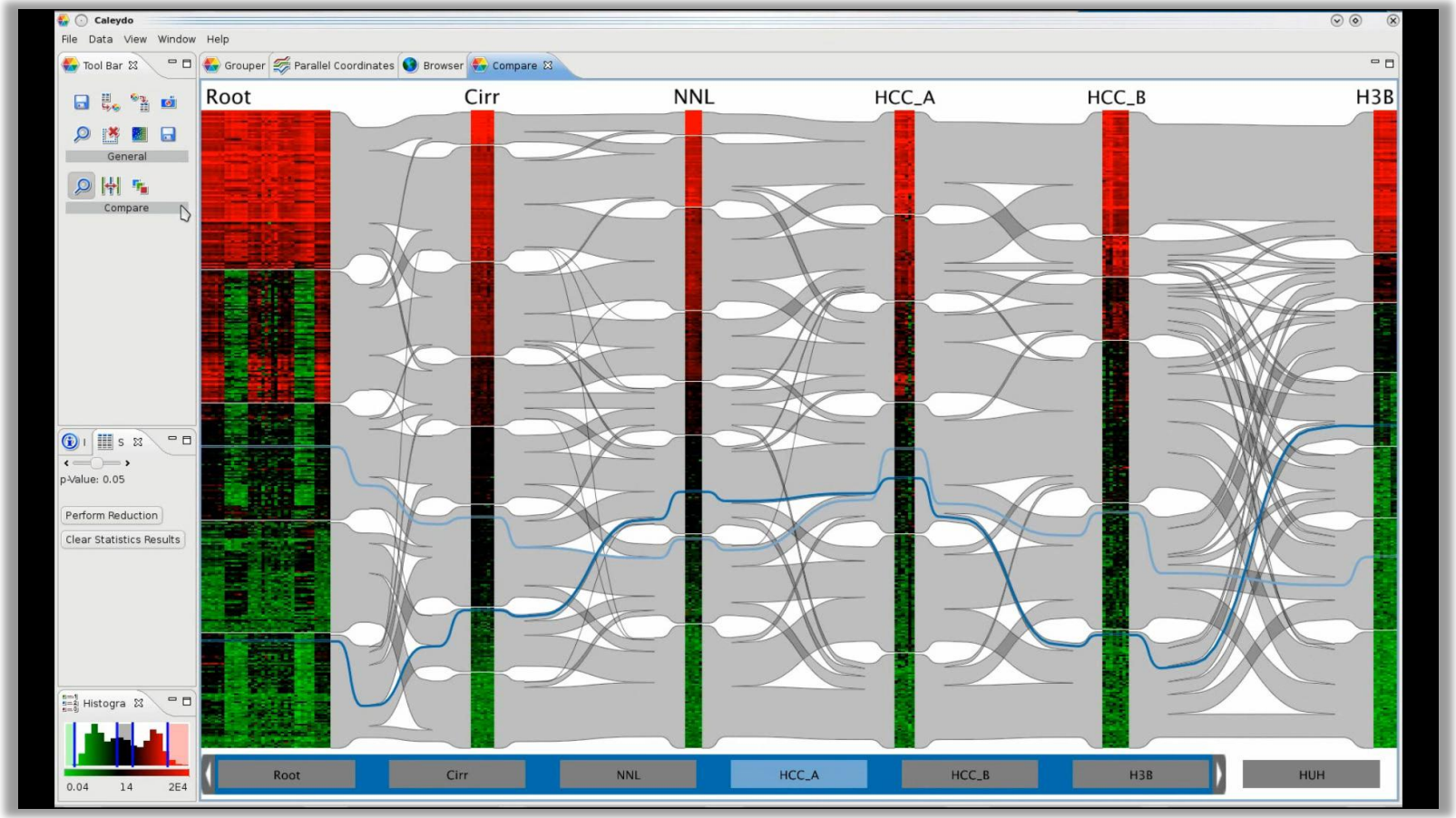


Using Splines



Using Pipes

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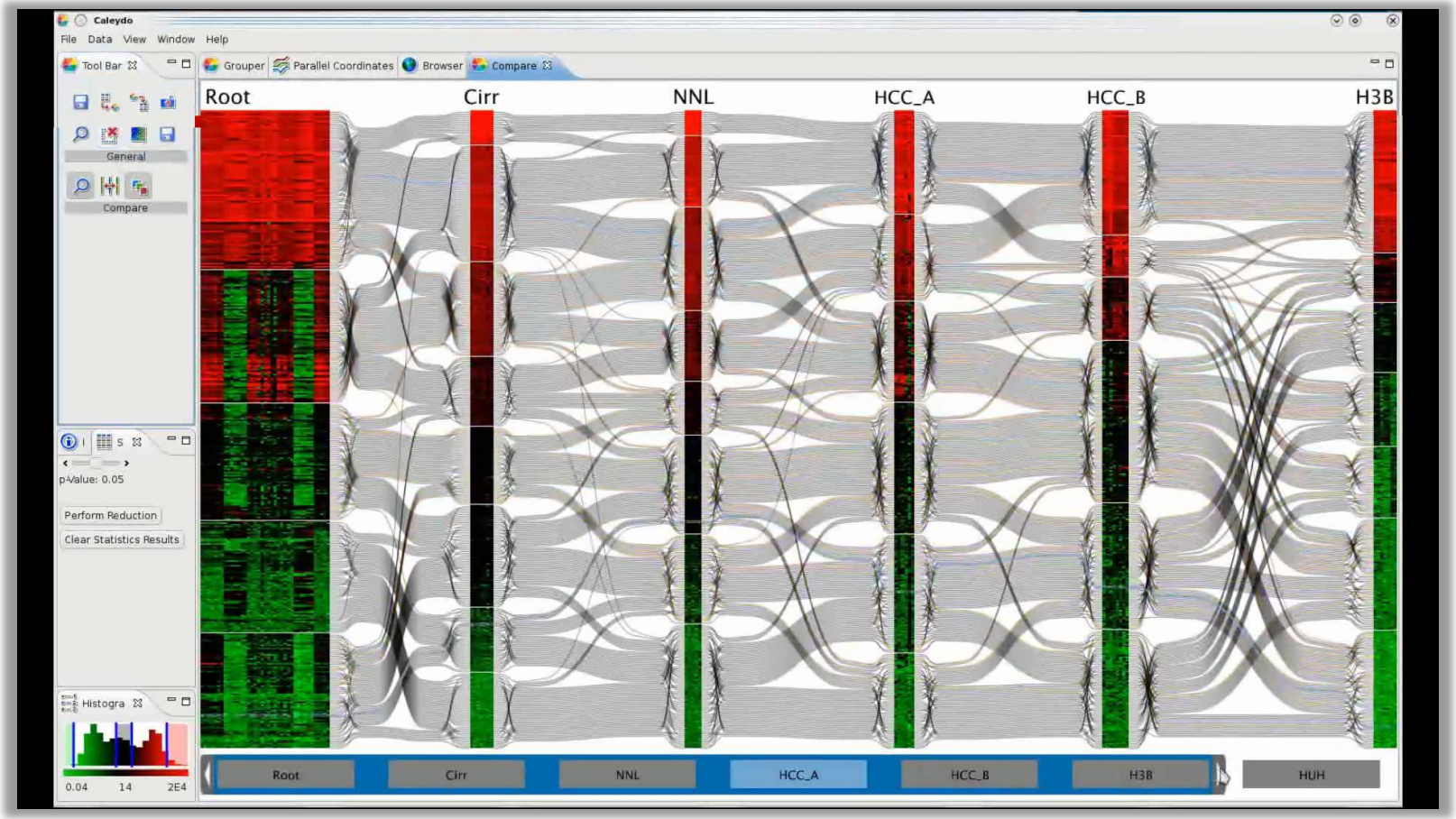
CALEYDO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Histogra
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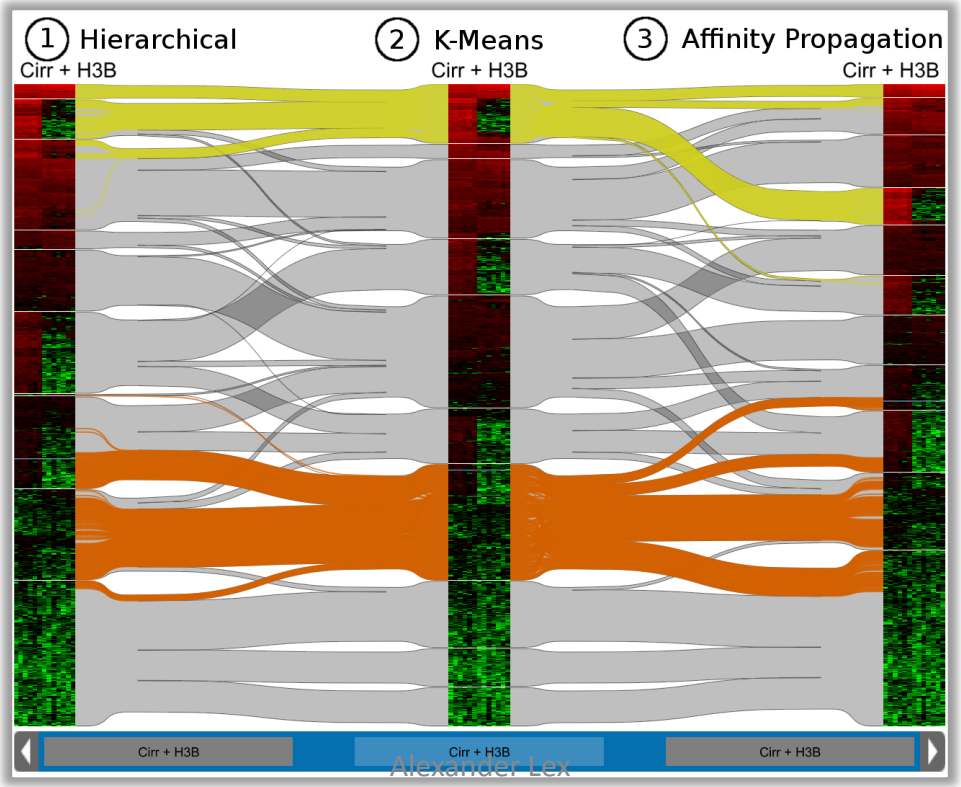
HCC_B
H3B
HUH

Example: Cluster Algorithm Comparison



CALEYDO

The next step: Abstraction

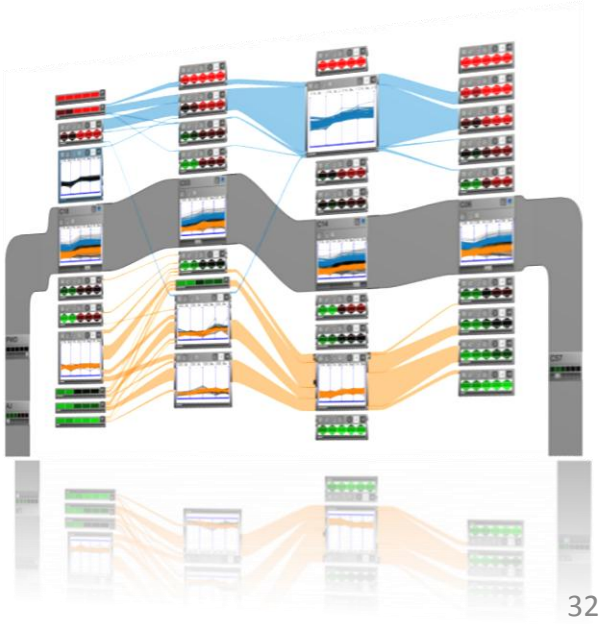
(Clustered) Datasets have homogeneous and inhomogeneous regions

No sense in wasting space for homogeneous parts

Use best visualization technique for each part and task!

[Lex, InfoVis 2011]

VISBRICKS



What is a Brick?

Shows part of data set

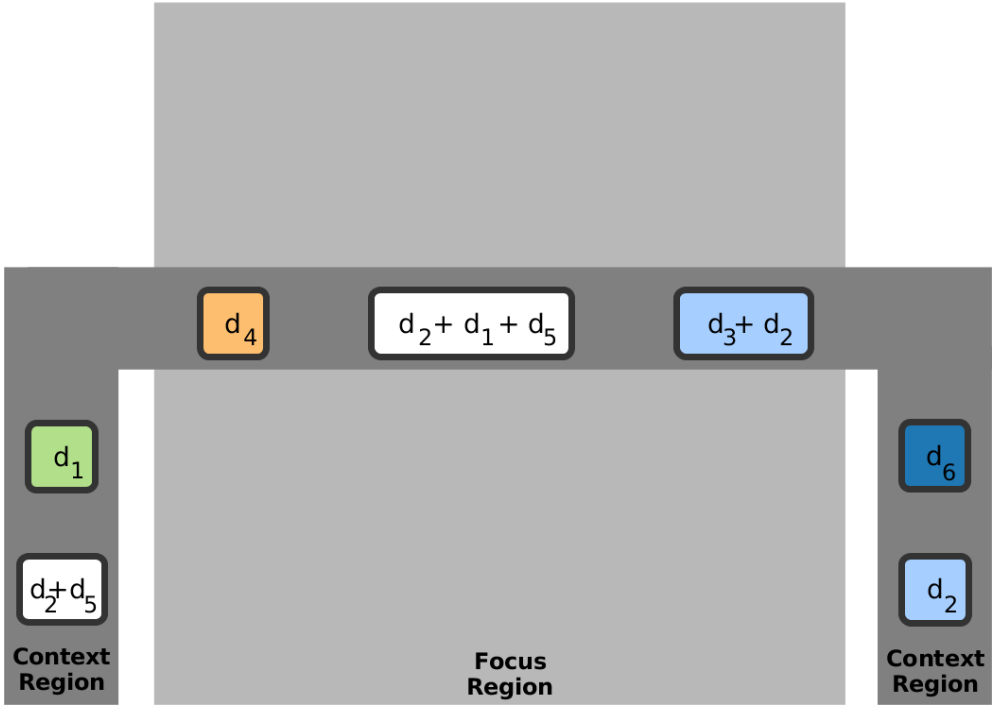
Multiform property:

- different levels of abstraction
- different visualization techniques

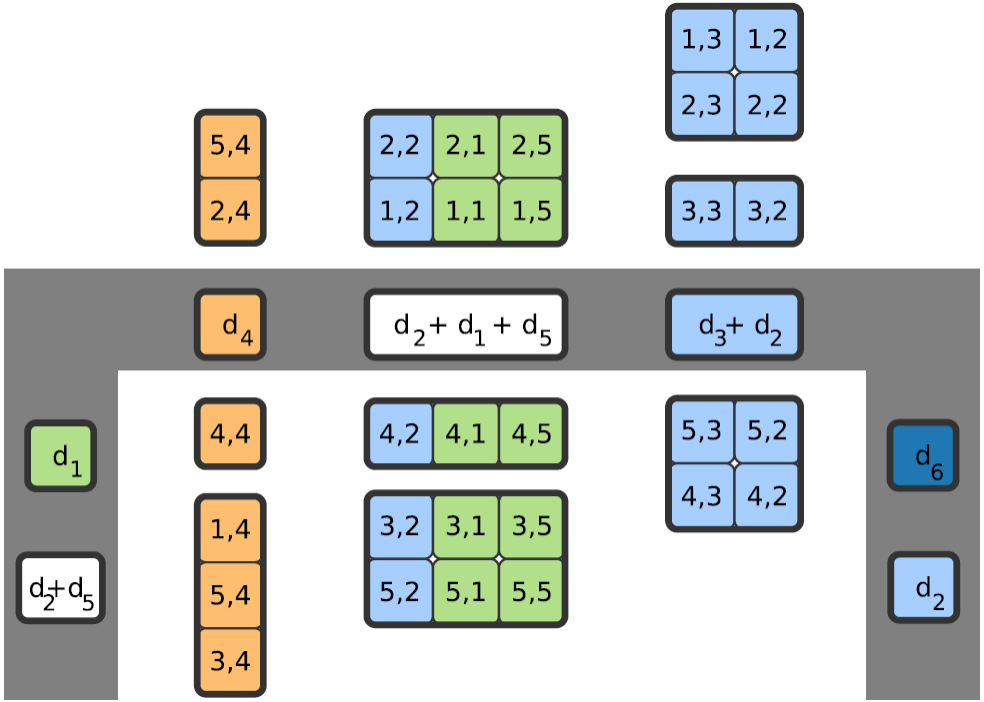
Two types of bricks:

- Dimension bricks
- Cluster bricks

Arrangement, Dimensions Bricks



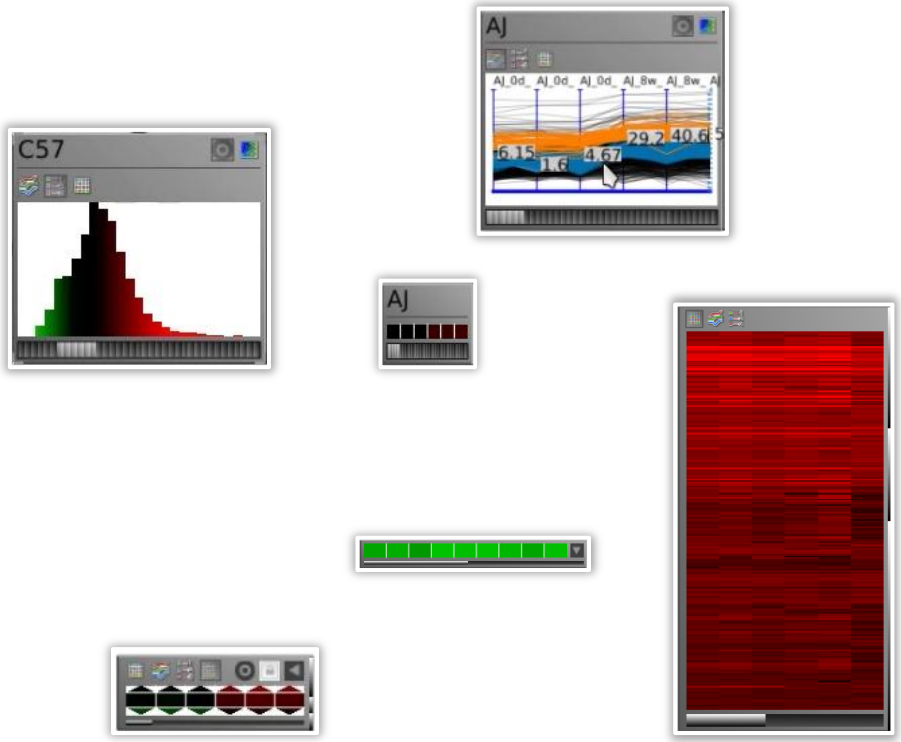
Added Cluster Bricks

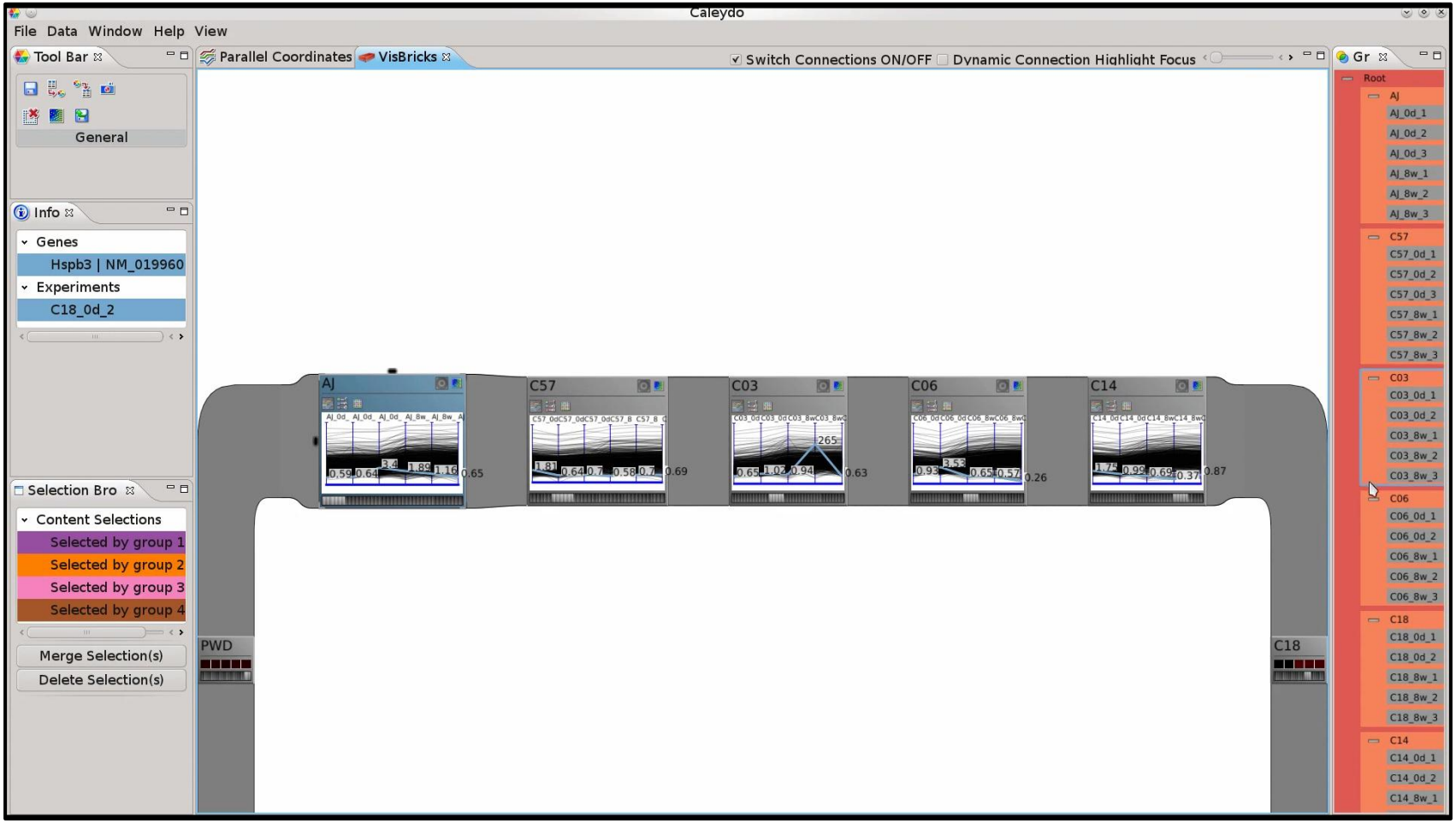


Examples for Bricks

Dimension Bricks

Cluster Bricks

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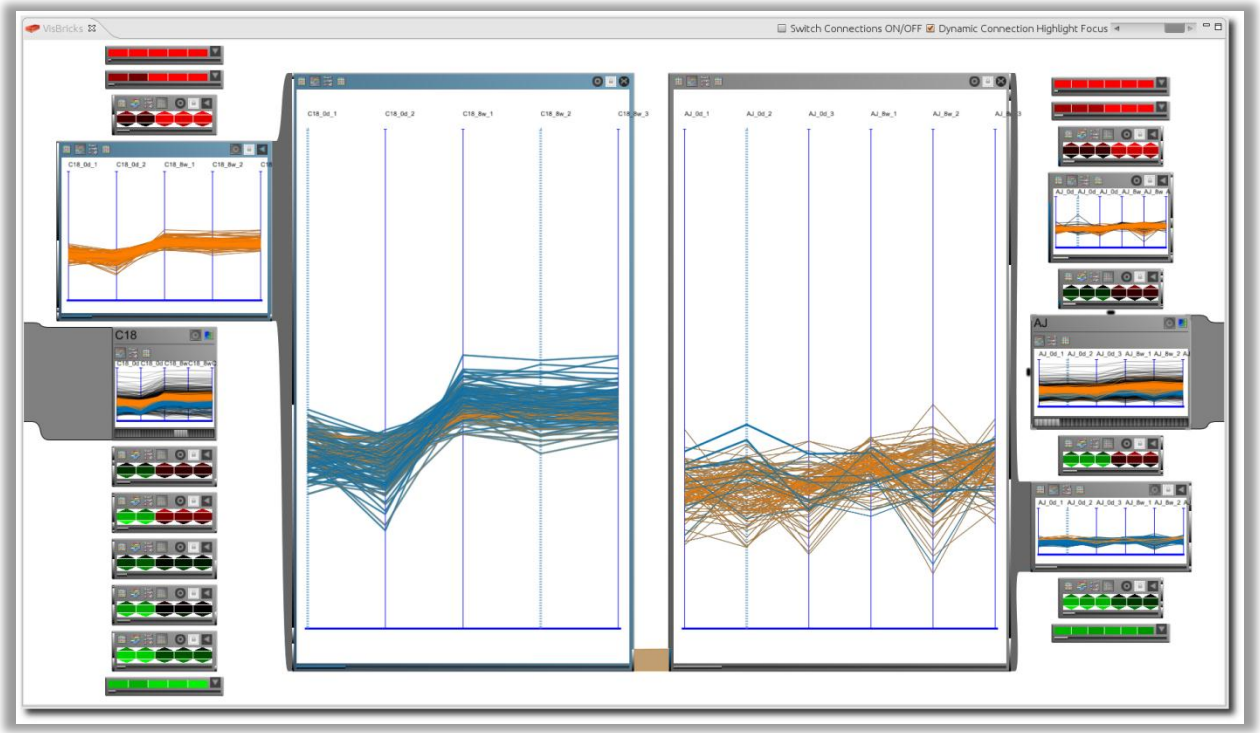
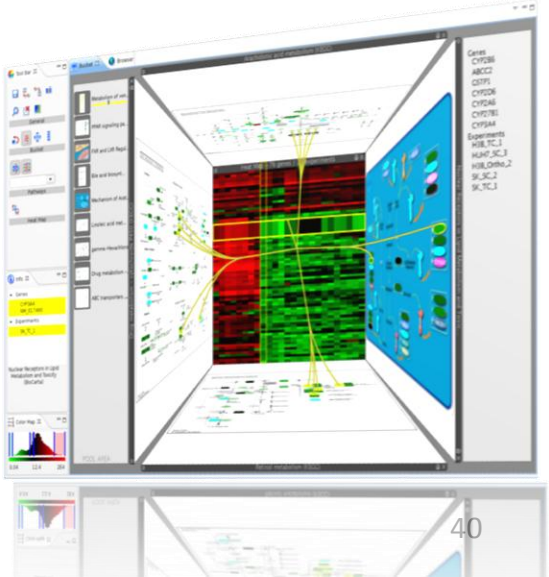
Exploring Details



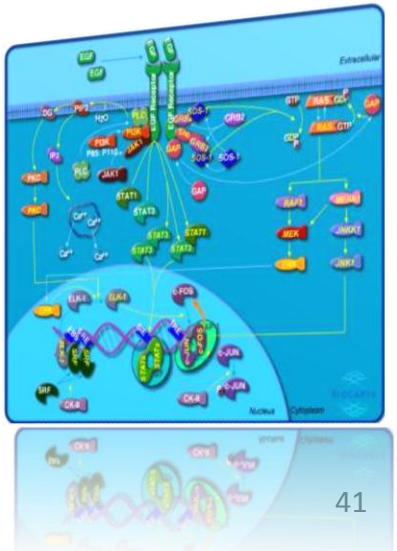
[Lex, PacificVis 2010]

PATHWAY EXPLORATION CALEYDO BUCKET

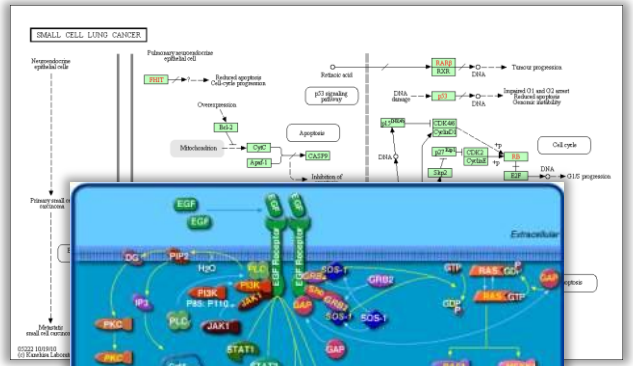


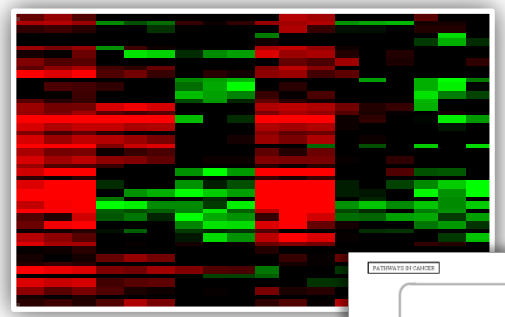
Pathway Visualization Goals

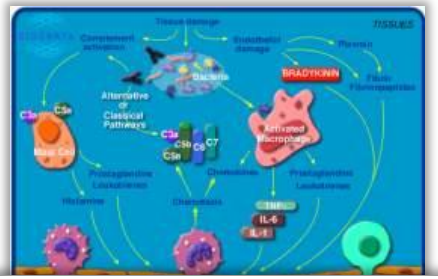
1. Map gene expression of multiple samples
2. Show the relations between pathways

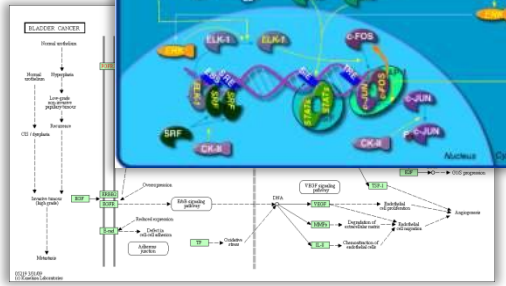


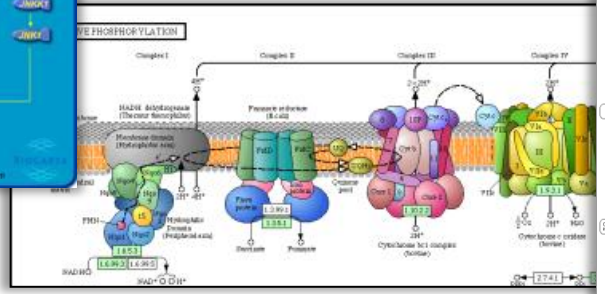
How to manage all these?

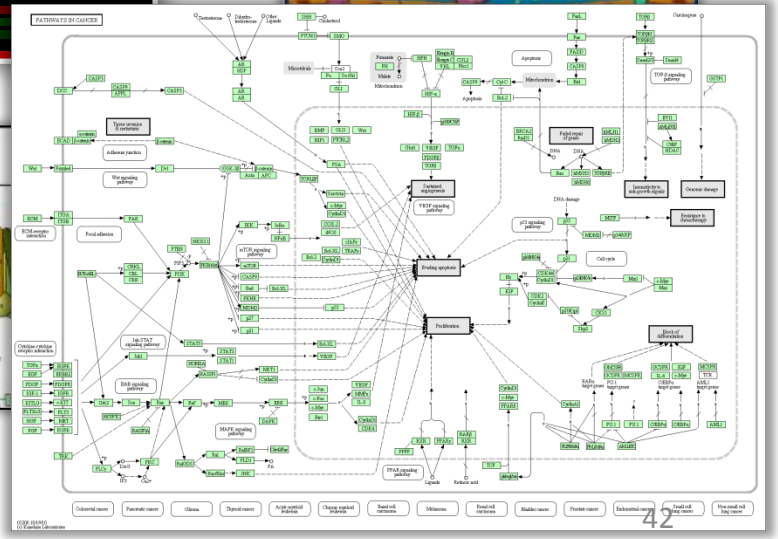




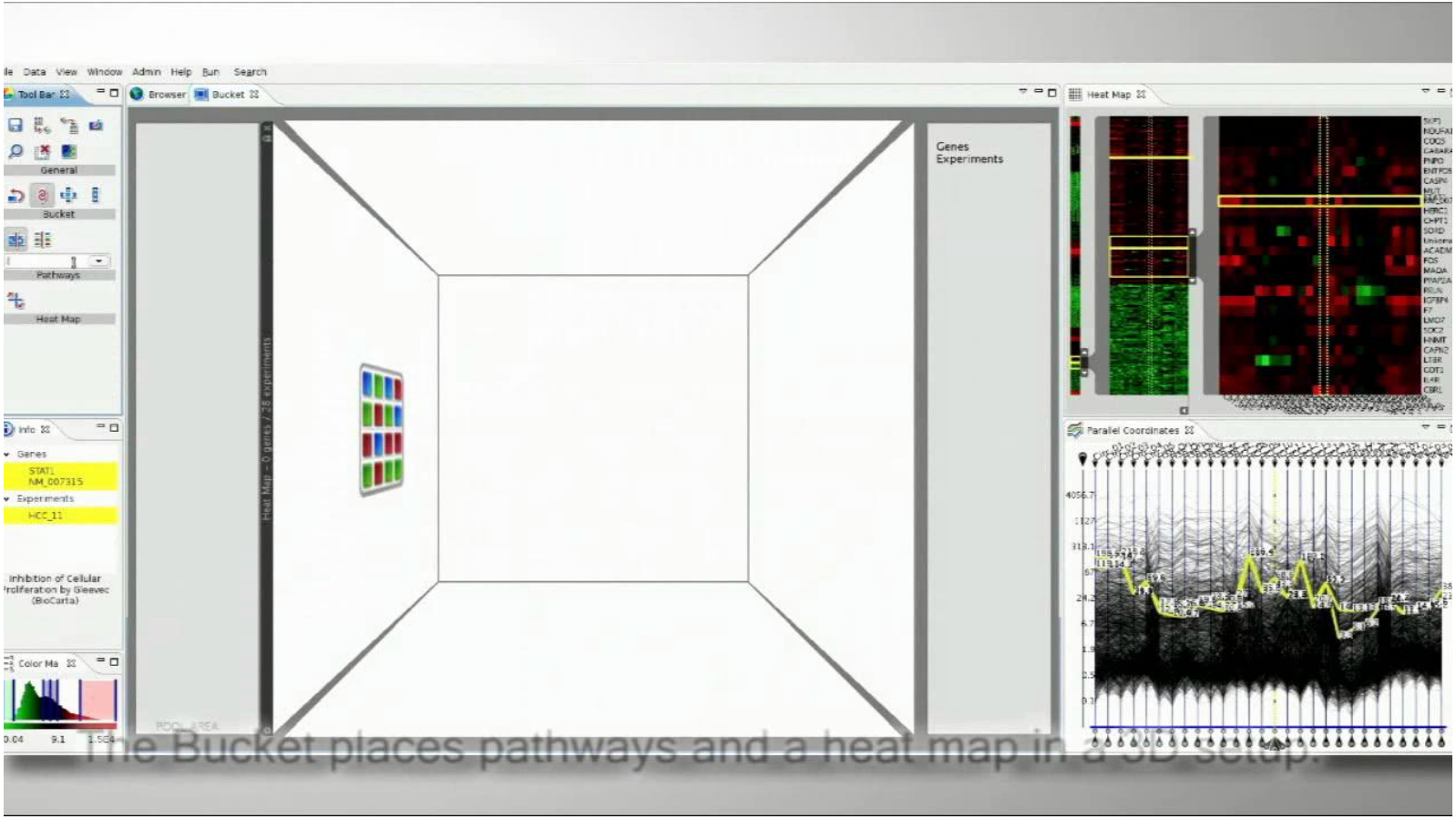








CALEYDO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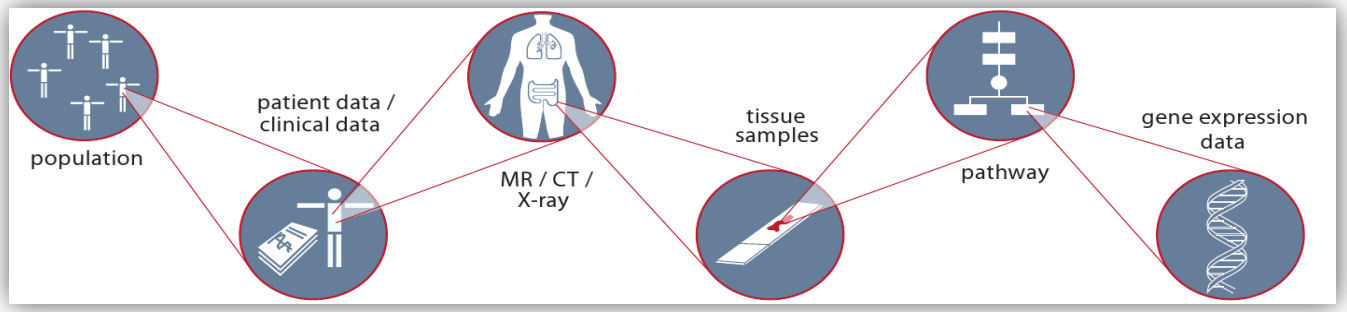
(BioCarta)
Color Ma
The Bucket places pathways and a heat map in a 3D setup.

CONNECTING HETEROGENEOUS DATA SETS

Research Topic 2

Heterogeneous Data Analysis

Massive amounts of data
Different abstraction levels
Different sources
Different formats

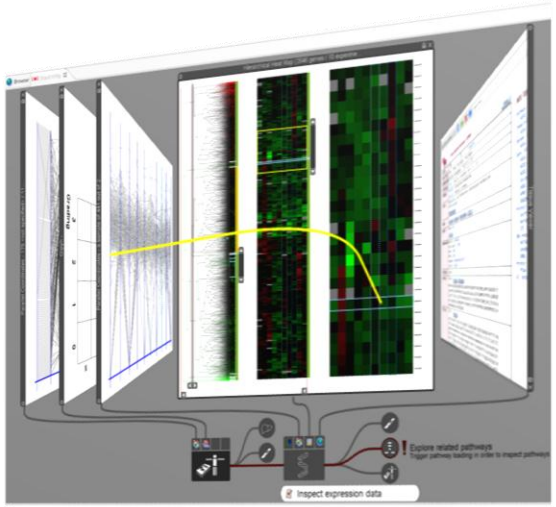


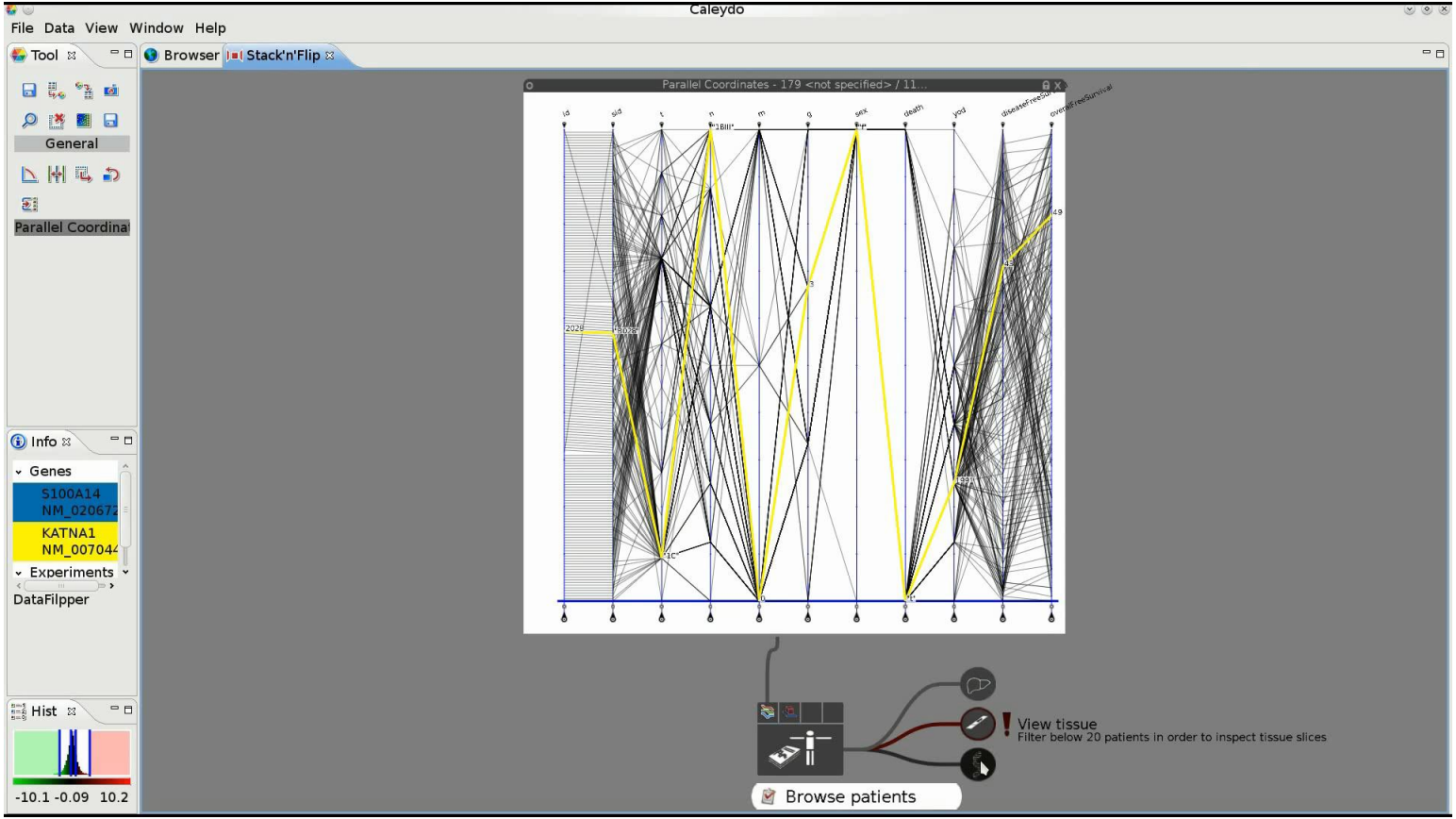
[Streit, CoVis 2009]

How to integrate data in a seamless analysis session?

[Streit, TVCG 2011]

GUIDANCE ACROSS MULTIPLE DATA SOURCES

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NM_007044
Experiments
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-10.1 -0.09 10.2
View tissue
Filter below 20 patients in order to inspect tissue slices
Browse patients

Super Application?

Expects a Super Application that can visualize everything

Not Feasible! Solution: use existing applications

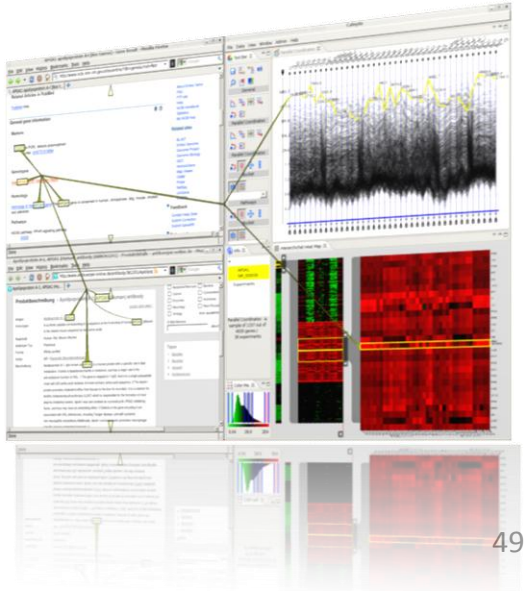
Downsides:

- not integrated
- no highlighting, linking, etc.

Can we solve this?

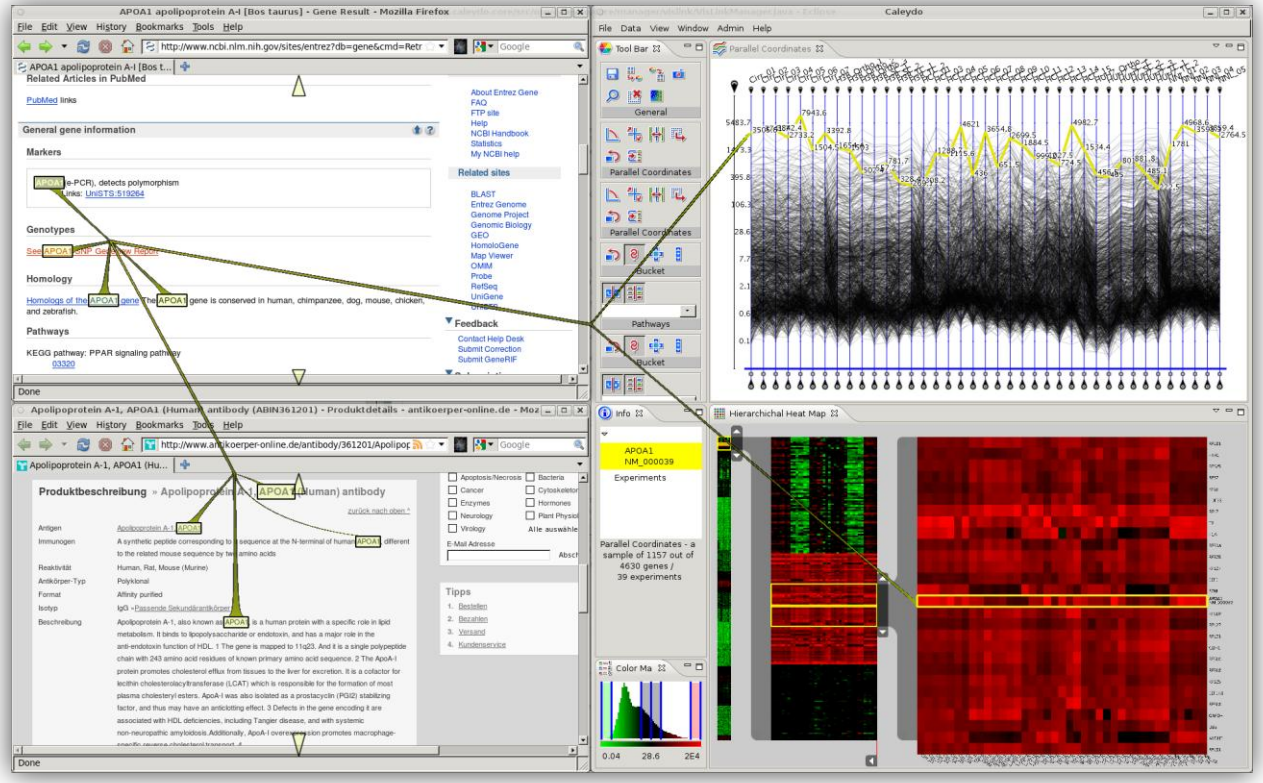
[Waldner, GI 2010] – best paper award

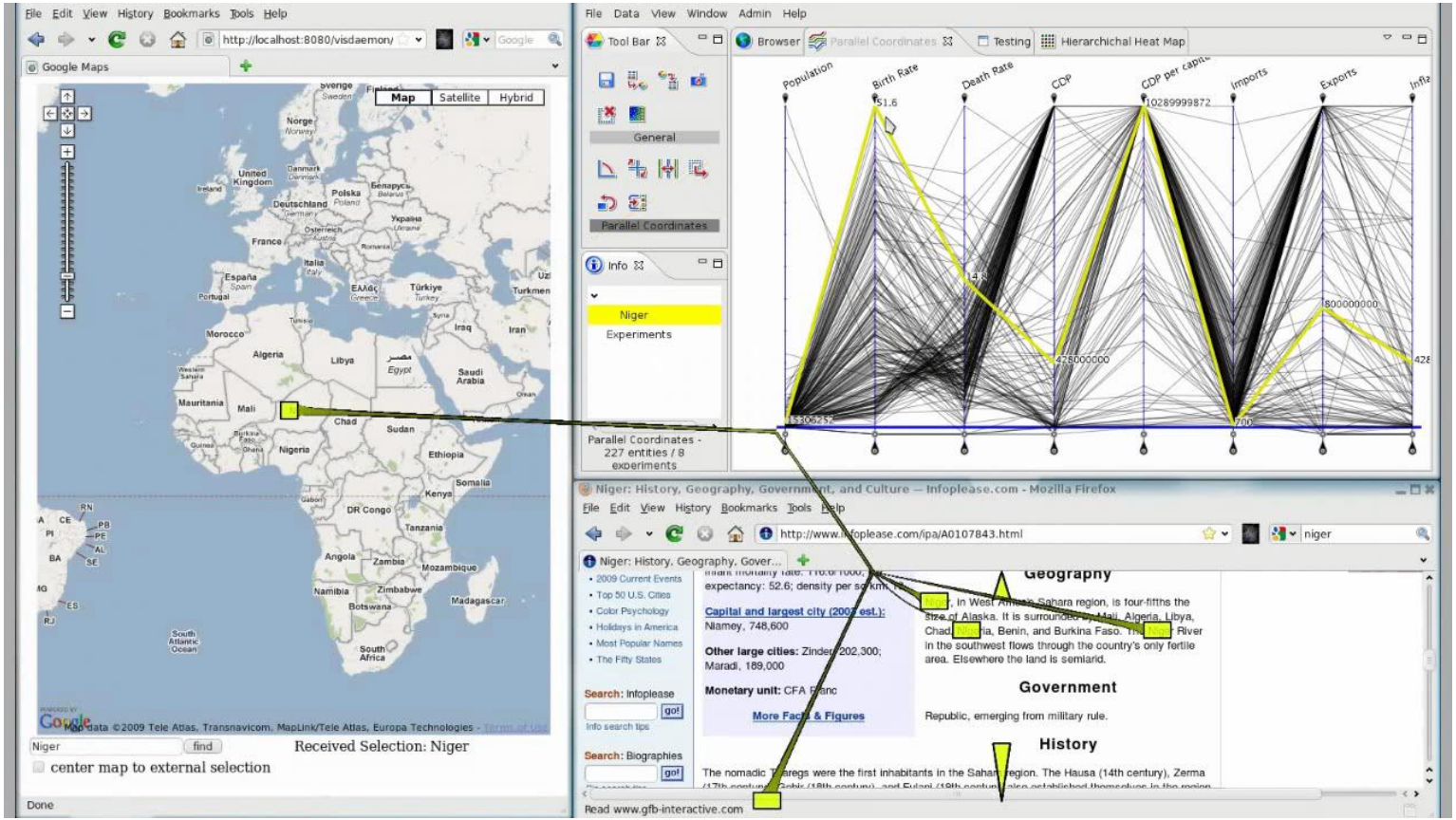
VISUAL LINKING ACROSS APPLICATIONS



CALEYDO

Visual Links Across Applications

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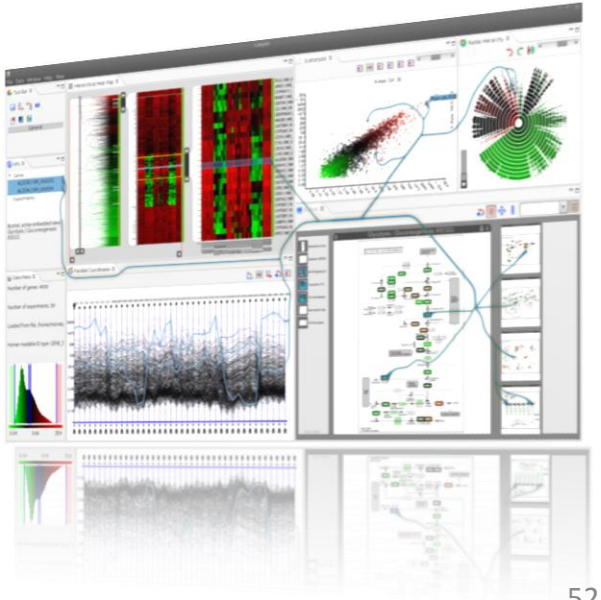
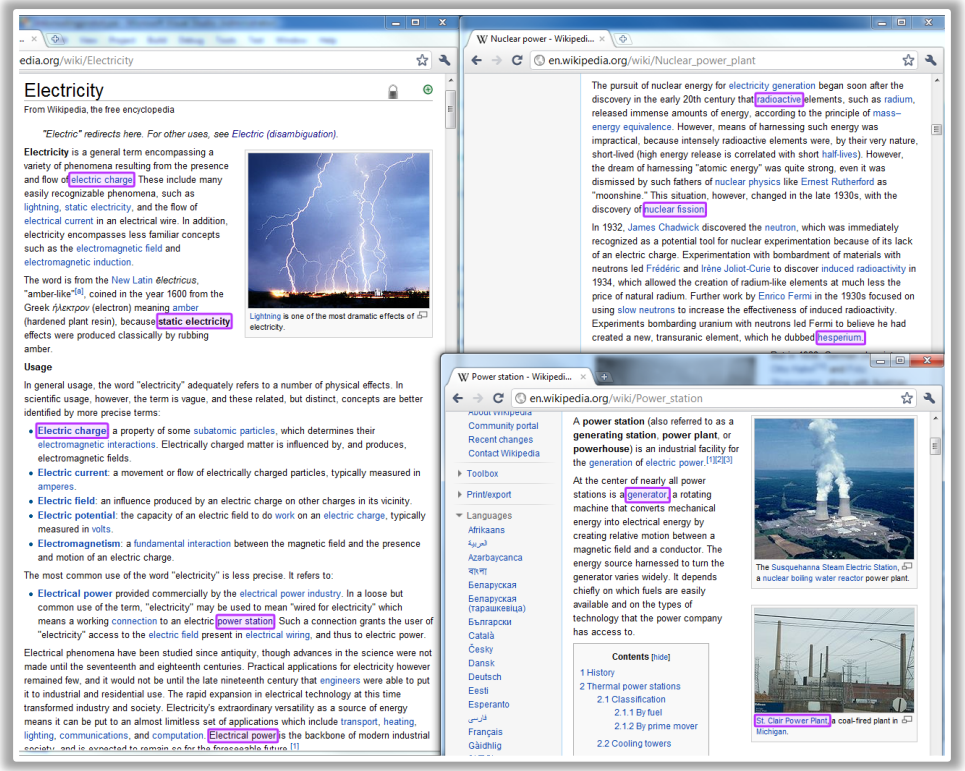
Map
Satellite
Hybrid
Received Selection: Niger
center map to external selection
Done
File Data View Window Admin Help
Tool Bar
General
Parallel Coordinates
Info
Niger
Experiments
Parallel Coordinates - 227 entities / 8 experiments
Browser
Parallel Coordinates
Testing
Hierarchichal Heat Map
Population
Birth Rate
Death Rate
GDP
Imports
Exports
51.6
10289999872
Niger: History, Geography, Government, and Culture — Infoplease.com - Mozilla Firefox
Capital and largest city (2007 est.):
Niamey, 748,600
Other large cities: Zinder 202,300; Maradi, 189,000
Monetary unit: CFA franc
More Facts & Figures
Geography
Government
Republic, emerging from military rule.
History
Read www.gfb-interactive.com

[Steinberger, InfoVis 2011]

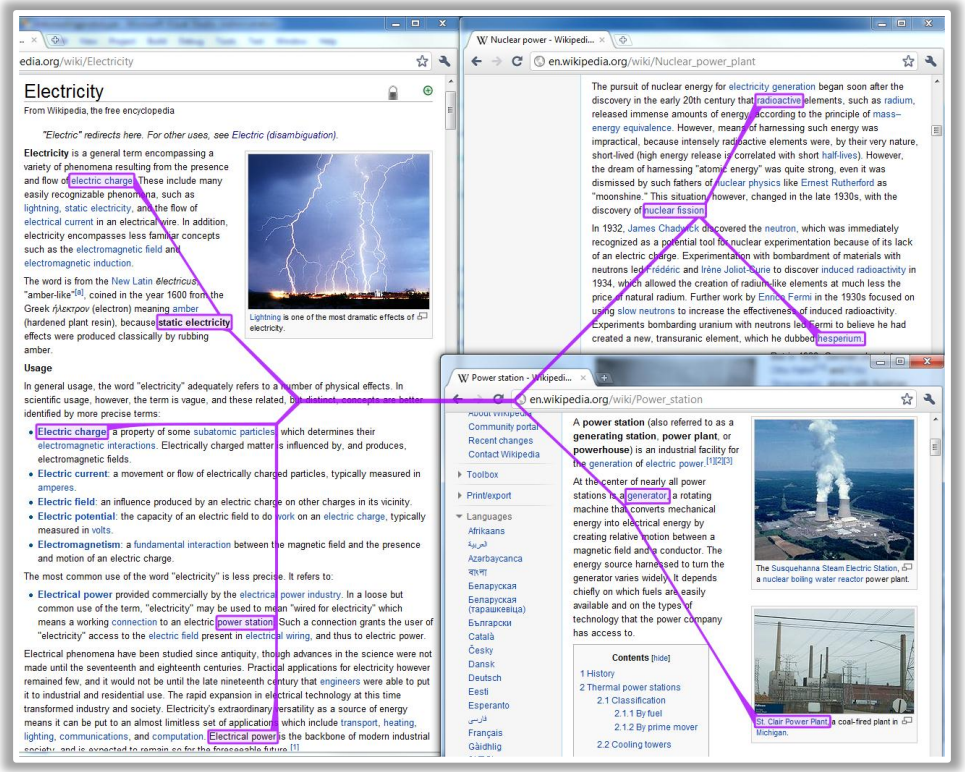
CONTEXT-AWARE VISUAL LINKS



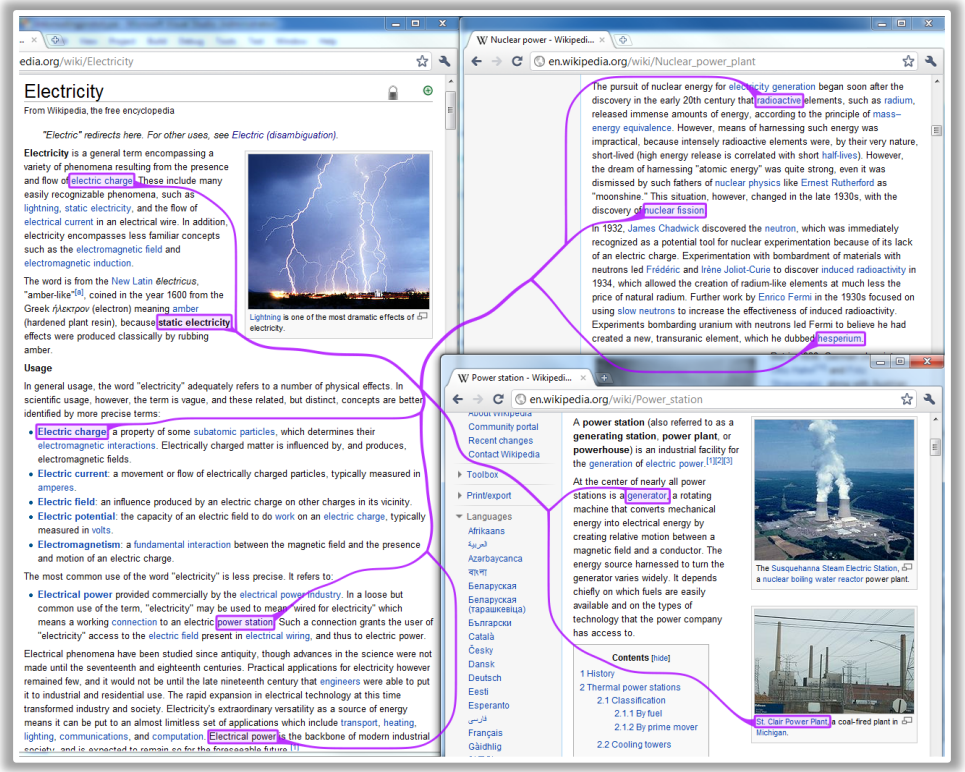
Simple Highlighting



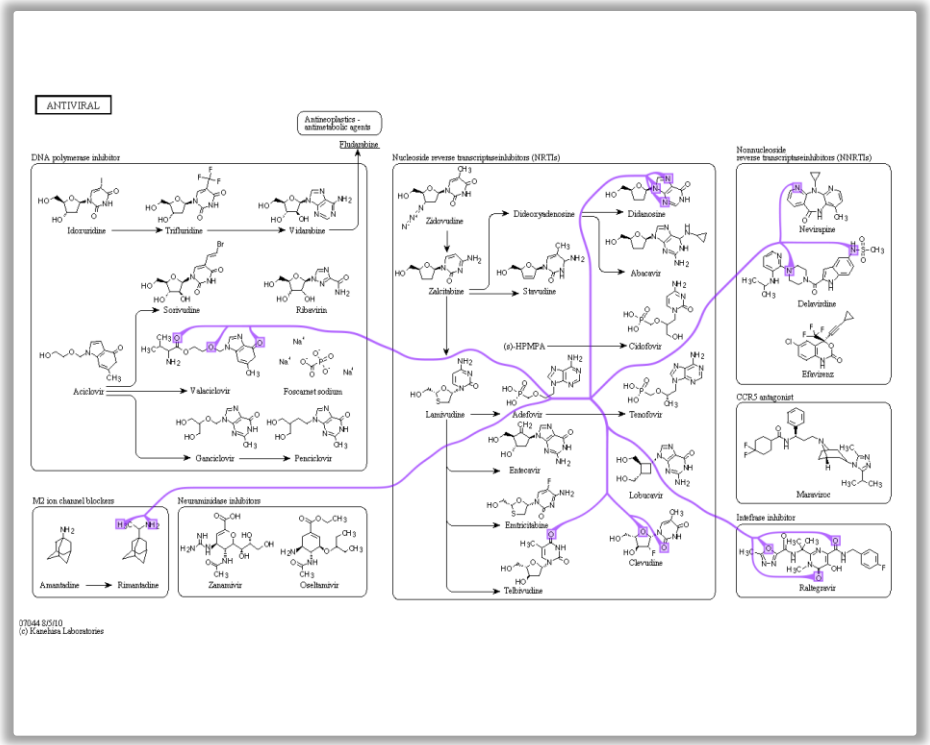
Traditional Visual Links



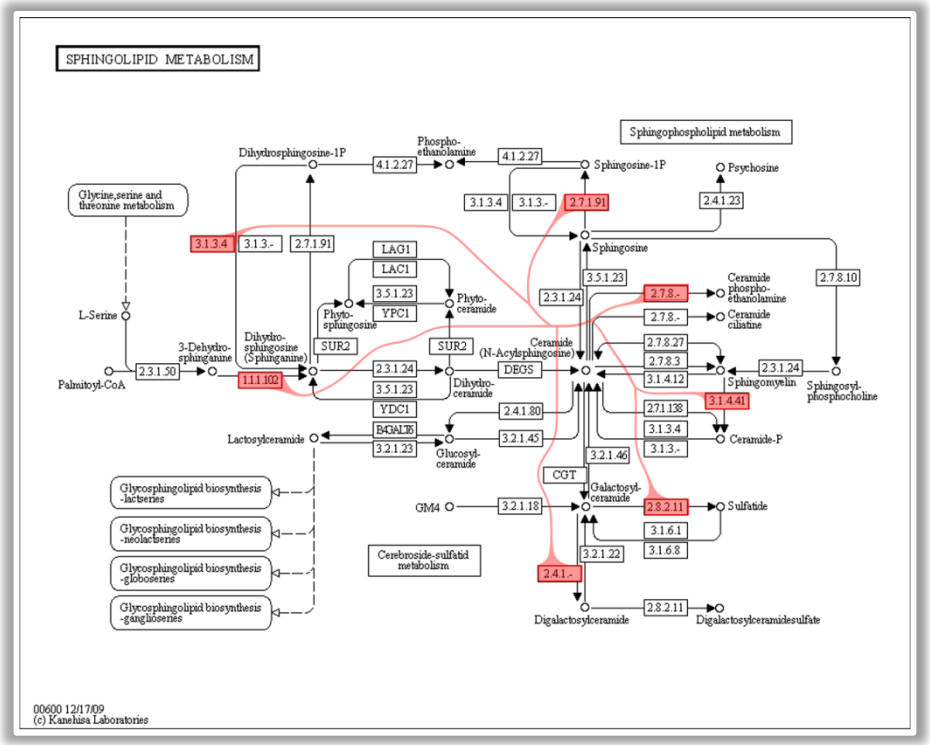
Context-Aware Visual Links



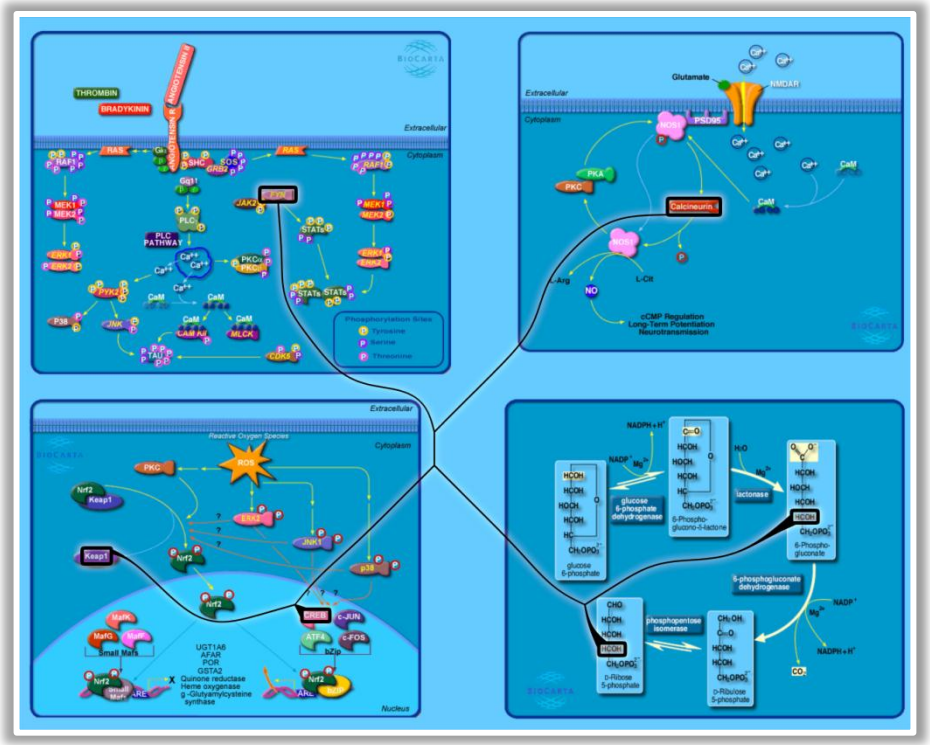
Kegg Pathway



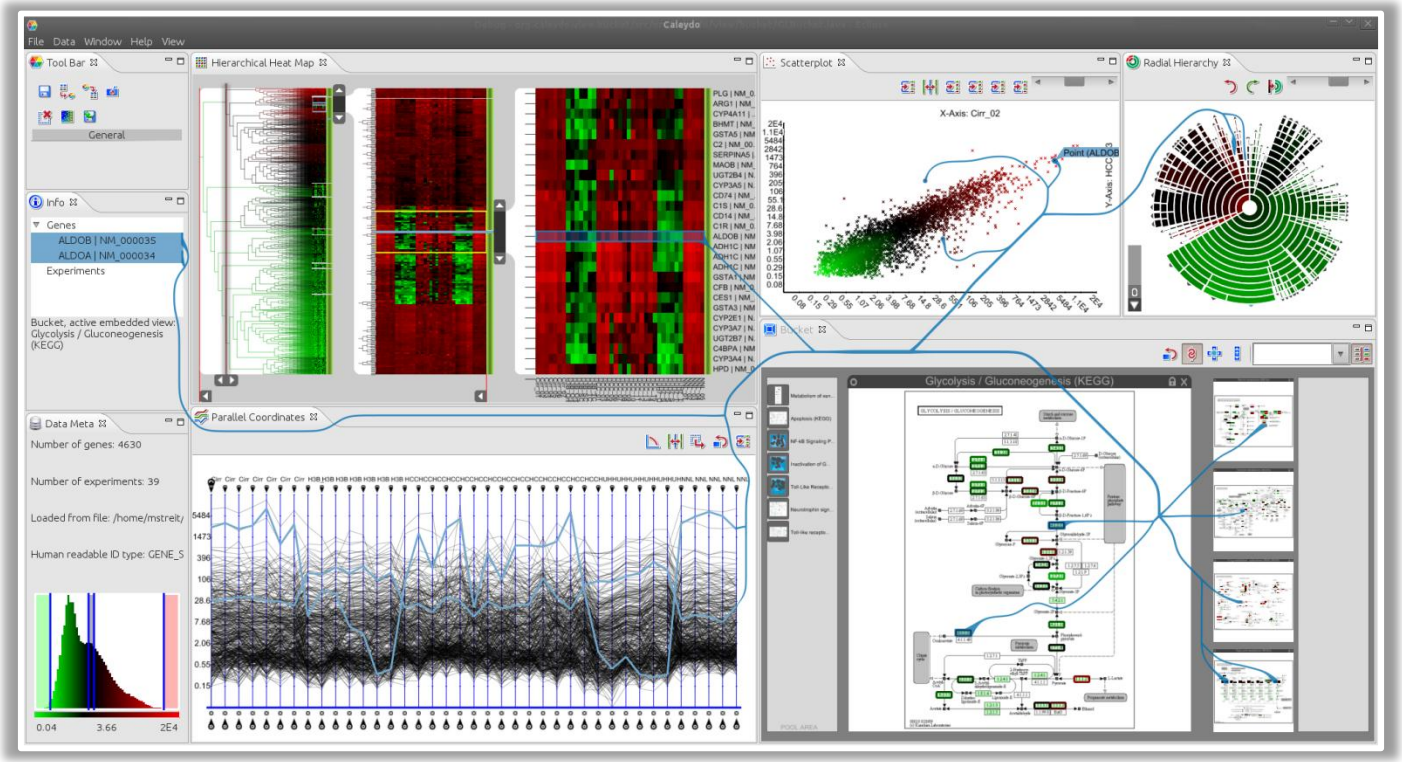
Kegg Pathway



Multiple Biocarta Pathways

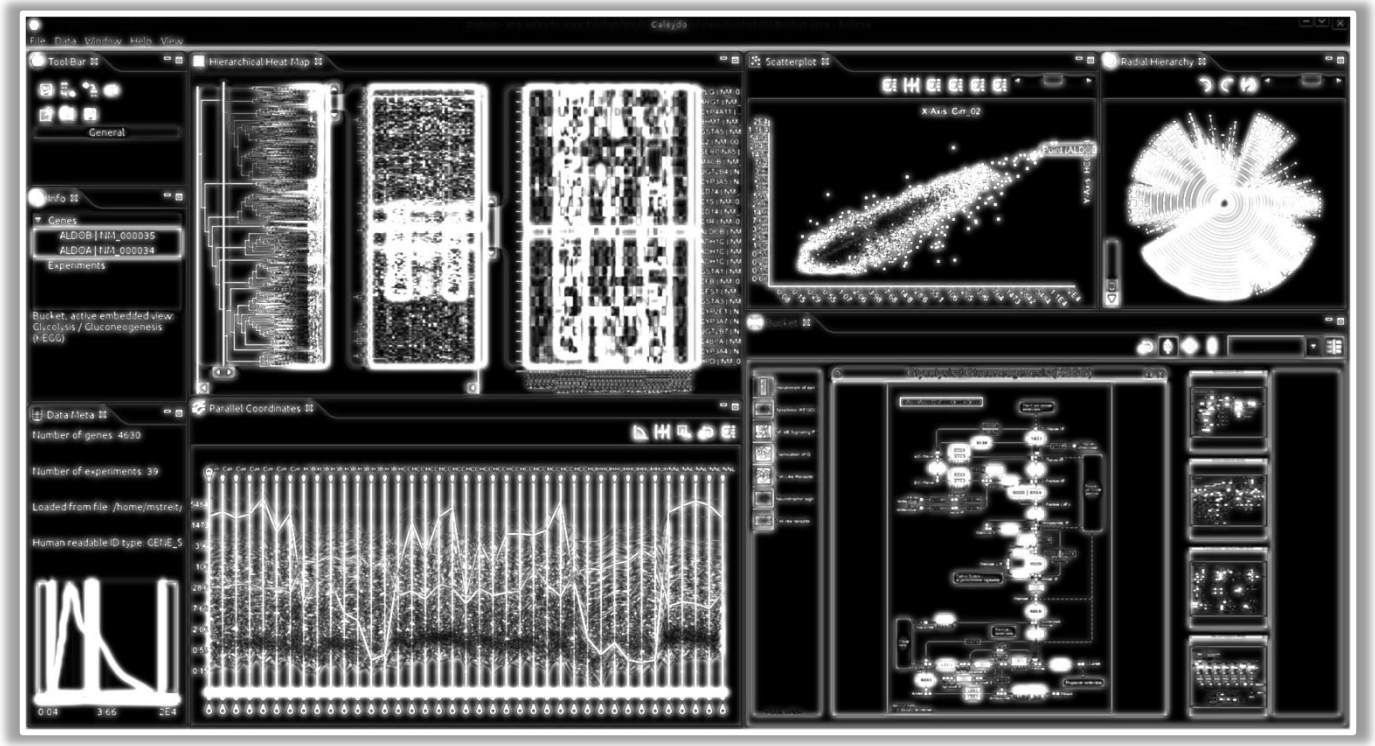


Caleydo

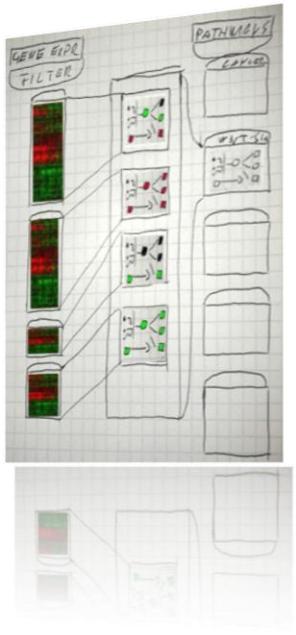


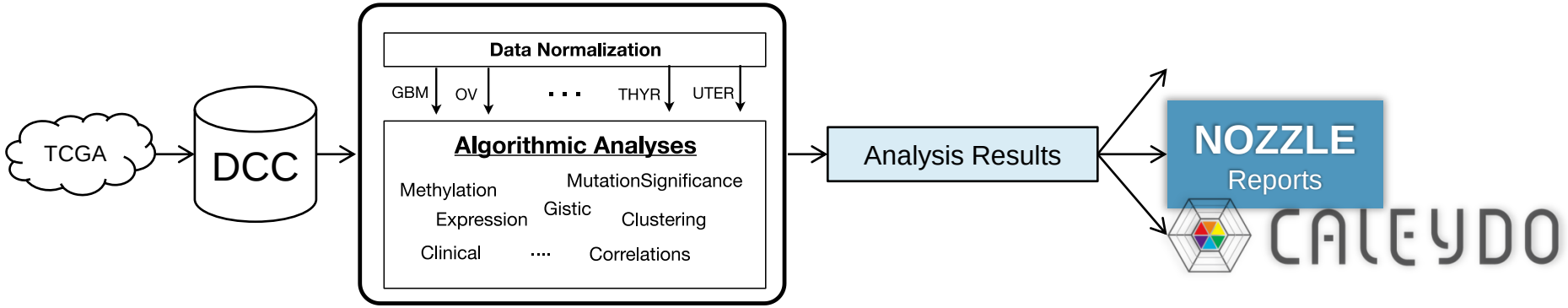
CALEYDO

How it works


Caleydo
File Data Window Help View
Tool Bar
General
Info
Genes
ALDOB | NM_000035
ALDOA | NM_000034
Experiments
Bucket, active embedded view:
Glycolysis / Gluconeogenesis
(4 EGO)
Data Meta
Number of genes: 4630
Number of experiments: 39
Loaded from file: /home/mstreit/
Human readable ID type: GENE_S
Hierarchical Heat Map
Parallel Coordinates
Scatterplot
X Axis: Cnt_02
Radial Hierarchy

PLANNED WORK HERE AT CBMI





Project Title Ideas:

OI – Omics Integrator

Frazzlomics

Wyee

Vision: Integrated Visualization of Multiple Datasets from Firehose

1. Analyze consistency of grouping

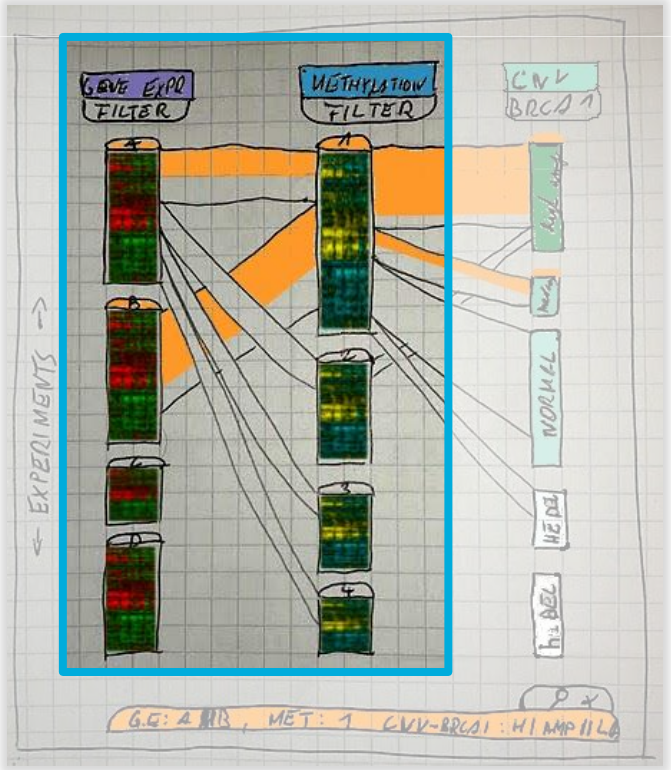
   across datasets

   between different results (e.g. 3 or 4 clusters?)

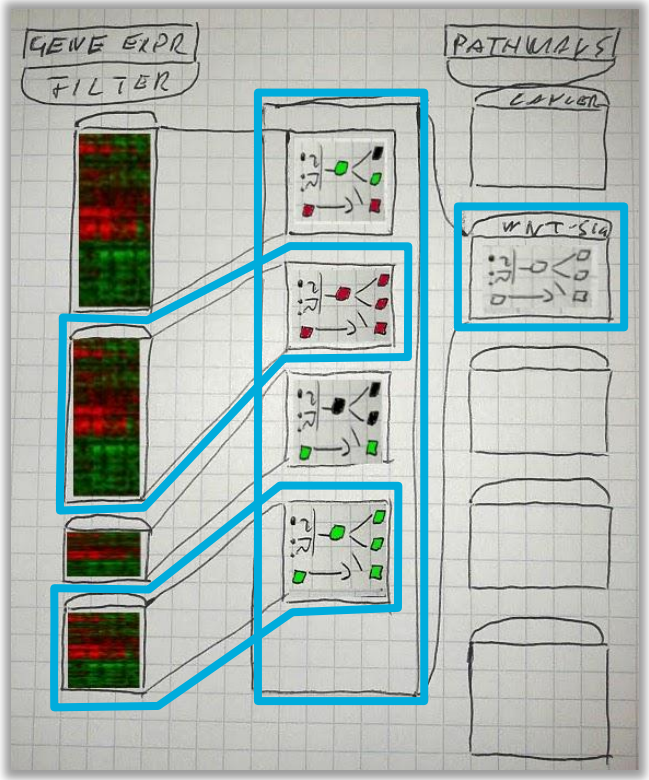
2. Analyze relations between grouping and structural variation data

3. Explore relations between pathways and groups

Showing Relationships



Integrating Pathways



Thank You!
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CALEYDO