Plug-and-Play Macroscopes That Empower Science

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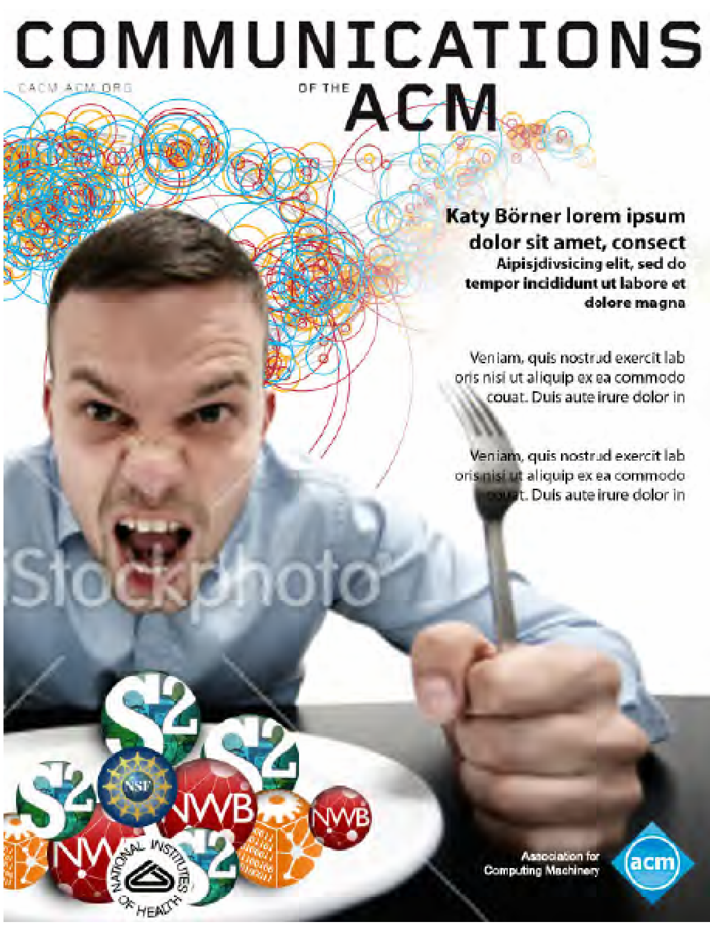
Center for Bioinformatics and Computational Biology
National Institute of General Medical Sciences, National Institutes of Health
Natcher 45, second floor, Room 2As.10

February 17, 2011



Börner, Katy. (March 2011). Plug-and-Play Macroscopes. *Communications of the ACM.*

Designing "Dream Tools"

Many of the best micro-, tele-, and macroscopes are designed by **scientists keen to observe and comprehend what no one has seen or understood before.** Galileo Galilei (1564–1642) recognized the potential of a spyglass for the study of the heavens, ground and polished his own lenses, and used the improved optical instruments to make discoveries like the moons of Jupiter, providing quantitative evidence for the Copernican theory.

Today, scientists **repurpose, extend, and invent new hardware and software** to create **"macroscopes"** that may solve both local and global challenges.

The tools I will show you today **empower** me, my students, colleagues, and 100,000 others that downloaded them.

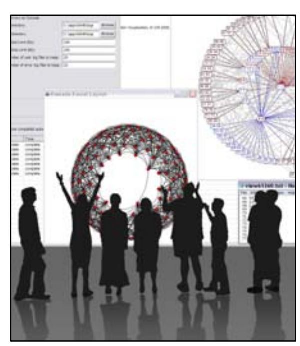
Macroscopes

Decision making in science, industry, and politics, as well as in daily life, requires that we make sense of data sets representing the structure and dynamics of complex systems. Analysis, navigation, and management of these continuously evolving data sets require a new kind of data-analysis and visualization tool we call a macroscope (from the Greek macros, or "great," and skopein, or "to observe") inspired by de Rosnay's futurist science writings.

Macroscopes provide a "vision of the whole," helping us "synthesize" the related elements and enabling us to detect patterns, trends, and outliers while granting access to myriad details. Rather than make things larger or smaller, **macroscopes let us observe what is at once too great, slow, or complex for the human eye and mind to notice and comprehend.**

Microscopes

Telescopes



Macroscopes

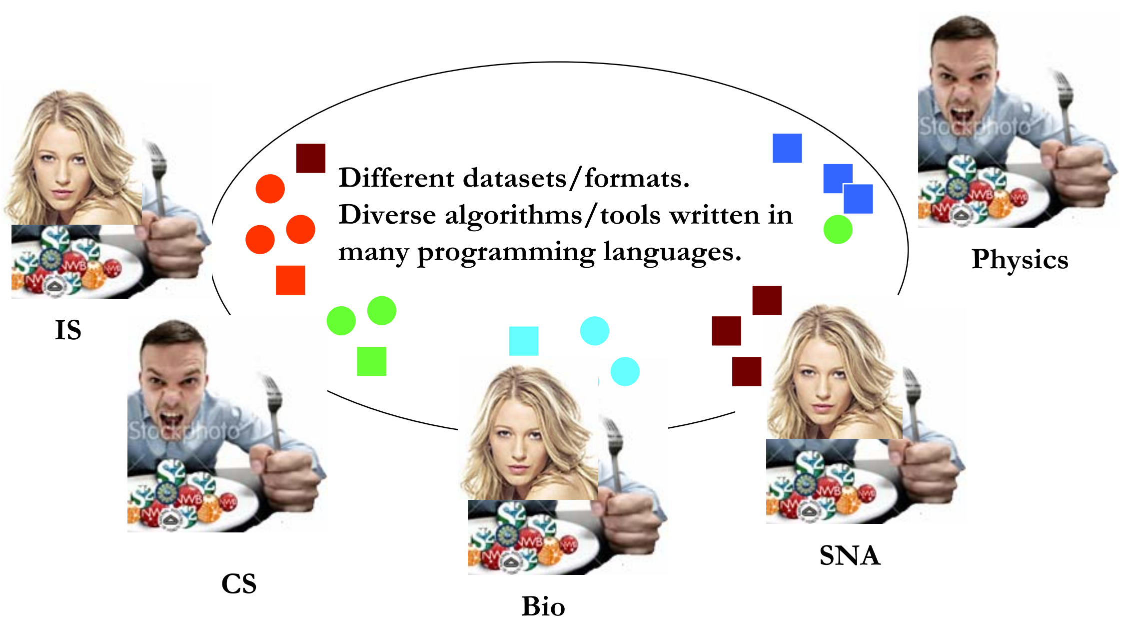
Goal of This Talk

Inspire computer scientists to implement software frameworks that **empower domain scientists** to assemble their own continuously evolving macroscopes, adding and upgrading existing (and removing obsolete) plug-ins to arrive at a set that is truly relevant for their work—with little or no help from computer scientists.

While microscopes and telescopes are physical instruments, **macroscopes resemble continuously changing bundles of software plug-ins.** Macroscopes make it easy to select and combine algorithm and tool plug-ins but also interface plug-ins, workflow support, logging, scheduling, and other plug-ins needed for scientifically rigorous yet effective work.

They make it easy to share plug-ins via email, flash drives, or online. To use new plugins, simply copy the files into the plug-in directory, and they appear in the tool menu ready for use. No restart of the tool is necessary. **Sharing algorithm components, tools, or novel interfaces becomes as easy as sharing images on Flickr or videos on YouTube. Assembling custom tools is as quick as compiling your custom music collection.**

Changing Scientific Landscape—Personal Observations



Changing Scientific Landscape—General Observations

Science becomes more data driven and computational but also collaborative and interdisciplinary. There is increased demand for tools that are easy to extend, share, and customize:

- *Star scientist —> Research teams.* Traditionally, science was driven by key scientists. Today, science is driven by collaborating co-author teams, often comprising experts from multiple disciplines and geospatial locations.
- *Users —> Contributors.* Web 2.0 technologies empower users to contribute to Wikipedia and exchange images, videos, and code via Fickr, YouTube, and SourceForge.net.
- *Disciplinary —> Cross-disciplinary.* The best tools frequently borrow and synergistically combine methods and techniques from different disciplines of science, empowering interdisciplinary and/or international teams to collectively fine-tune and interpret results;
- *Single specimen —> Data streams.* Microscopes and telescopes were originally used to study a single specimen at a time. Today, many researchers must make sense of massive data streams comprising multiple data types and formats from different origins; and
- *Static instrument —> Evolving cyberinfrastructure.* The importance of hardware instruments that are static and expensive tends to decrease relative to software tools and services that are highly flexible and evolving to meet the needs of different sciences. Some of the most successful tools and services are decentralized, increasing scalability and fault tolerance.

Related Work

Google Code and SourceForge.net provide special means for developing and distributing software

- In August 2009, SourceForge.net hosted more than 230,000 software projects by two million registered users (285,957 in January 2011);
- In August 2009 ProgrammableWeb.com hosted 1,366 application programming interfaces (APIs) and 4,092 mashups (2,699 APIs and 5,493 mashups in January 2011)

Cyberinfrastructures serving large biomedical communities

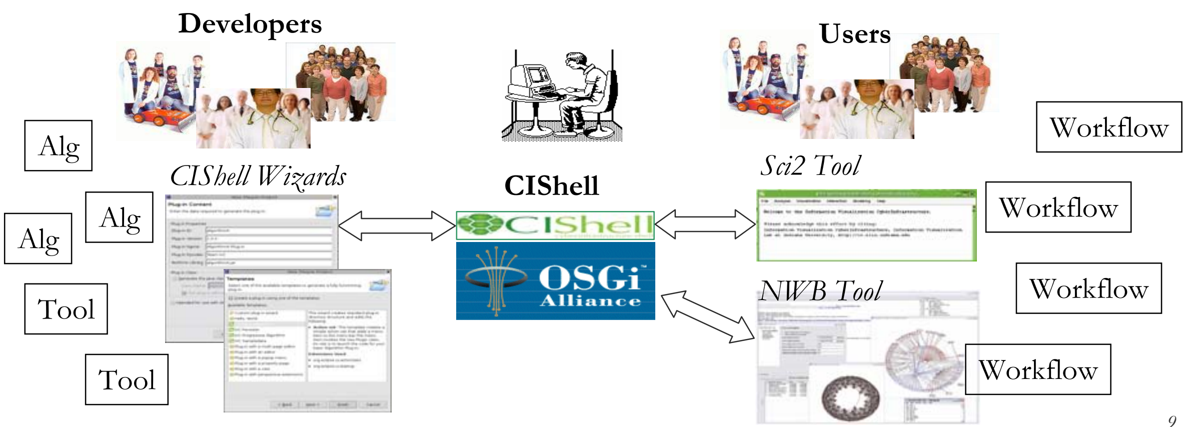
- Cancer Biomedical Informatics Grid (caBIG) (http://cabig.nci.nih.gov)
- Biomedical Informatics Research Network (BIRN) (http://nbirn.net)
- Informatics for Integrating Biology and the Bedside (i2b2) (https://www.i2b2.org)
- HUBzero (http://hubzero.org) platform for scientific collaboration uses
- myExperiment (http://myexperiment.org) supports the sharing of scientific workflows and other research objects.

Missing so far is a **common standard** for

- the design of **modular, compatible algorithm and tool plug-ins** (also called "modules" or "components")
- that can be **easily combined into scientific workflows** ("pipeline" or "composition"),
- and packaged as **custom tools.**

OSGi & CIShell

- CIShell (http://cishell.org) is an open source software specification for the integration and utilization of datasets, algorithms, and tools.
- It extends the Open Services Gateway Initiative (OSGi) (http://osgi.org), a standardized, component oriented, computing environment for networked services widely used in industry since more than 10 years.
- Specifically, CIShell provides "sockets" into which existing and new datasets, algorithms, and tools can be plugged using a wizard-driven process.



CIShell Features

A framework for easy integration of new and existing algorithms written in any programming language Using CIShell, an algorithm writer can fully concentrate on creating their own algorithm in whatever language they are comfortable with. Simple tools are provided to then take their algorithm and integrate it into cishell with no additional coding.

A well-defined pool of algorithms and datasets CIShell clearly defines how algorithms and datasets are integrated into the system to create a pool of algorithms and data. An application may then query for algorithms in this pool and execute them. Many applications/tools can be built and customized for different user groups by utilizing the same pool of algorithms.

Leveraging open standards CIShell avoids re-inventing wheels by building on other standards for its specification and reference implementations. It benefits most from the **Eclipse** family of projects (in particular, the **Rich Client Platform** and **Equinox**) and the Open Services Gateway Initiative (**OSGi**). All CIShell algorithms are integrated as OSGi services and can be used by any OSGi compliant system (including any Eclipse 3.0 or newer based products).

Choose the way you work CIShell offers reference applications that build on the pool of algorithms defined by CIShell. Scripting and a Graphical User Interface (GUI) are offered initially with a remoting (peer-to-peer and client-server) architecture, a web front-end, and other interfaces planned. We invite other toolkit developers to build their own applications on top of CIShell's algorithm pool.

Open source, community-driven project

CIShell is released under the Apache 2.0 License. Community input is welcome to create a piece of software that advances science and education.

CIShell Developer Guide
(*http://cishell.org/?n=DevGuide.NewGuide* soon at *http://cishell.wiki.cns.iu.edu*)

Algorithm Developer's Guide

Overview

The Cyberinfrastructure Shell (CIShell) is an open source, community-driven platform for the integration and utilization of datasets, algorithms, tools, and computing resources. Algorithm integration support is built in for Java and most other programming languages. Being Java based, it will run on almost all platforms. The software and specification is released under an Apache 2.0 License.

This guide attempts to aid algorithm developers in creating algorithms for CIShell (and applications built on CIShell).

This guide tries to contain all the information a new developer needs, but where necessary, it may cite the CIShell 1.0 Specification (API) or the OSGi Service Platform Specification, Release 4 (API). While the guide tries to make beginning algorithm development easier, the CIShell Specification has the last word on how the CIShell Platform works.

Table of Contents

CIShell Portal (http://cishell.org/home.html)


CIShell Powered
Tools Portal

Cyberinfrastructure Shell (CIShell)
CIShell supports the plug-and-play of datasets and algorithms and their bundling into custom tools that serve the specific needs of a user group or research community. It has been applied to develop diverse custom tools, see below. Feel free to take plugins from any of these tools to design your personal dream tool.

Visit the CIShell wiki to learn more about using CIShell as a platform for your tool!

Provided by the Cyberinfrastructure for Network Science Center at Indiana University.

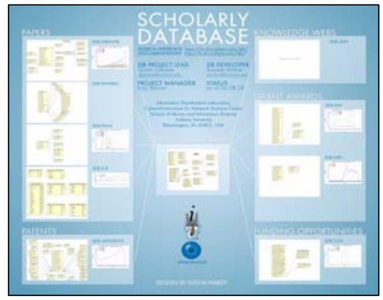
Learn more about existing CIShell-powered tools below.

Network Workbench Tool (NWB)
The NWB Tool supports researchers, educators, and practitioners interested in the study of biomedical, social and behavioral science, physics, and other networks. It comes with a 77-page user manual.

Gallery

Science of Science Tool (Sci^2)
The Sci^2 Tool was specifically developed for science policy makers and researchers that study science by scientific means. It supports the temporal, geospatial, topical, and network analysis and visualization of scholarly datasets at the micro (individual), meso (local), and macro (global) levels. There exists a 112-page user manual and 24 hours of NIH tutorials in this tool.

Science of Science Cyberinfrastructures



Scholarly Database: 25 million scholarly records
http://sdb.slis.indiana.edu

James S. McDonnell Foundation

VIVO Research Networking
http://vivoweb.org

Information Visualization Cyberinfrastructure
http://iv.slis.indiana.edu

Network Workbench Tool & Community Wiki
http://nwb.slis.indiana.edu

Science of Science (Sci²) Tool and CI Portal
http://sci.slis.indiana.edu

Epidemics Cyberinfrastructure
http://epic.slis.indiana.edu/

OSGi Alliance

CIShell
cyberinfrastructure shell

NetworkWorkbench
A Workbench for Network Scientists

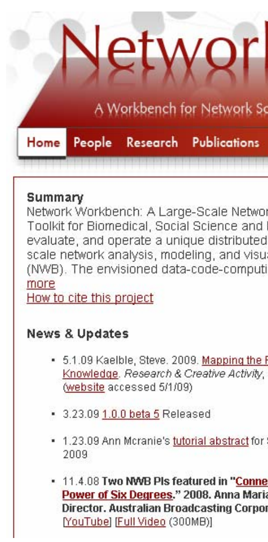
Network Workbench Tool
http://nwb.slis.indiana.edu

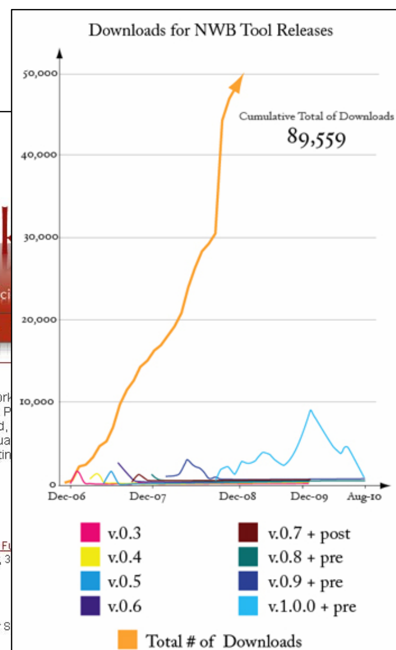
The Network Workbench (NWB) tool supports researchers, educators, and practitioners interested in the study of biomedical, social and behavioral science, physics, and other networks.

In February 2009, the tool provides more 169 plugins that support the preprocessing, analysis, modeling, and visualization of networks.

More than 50 of these plugins can be applied or were specifically designed for S&T studies.

It has been downloaded more than 65,000 times since December 2006.





Herr II, Bruce W., Huang, Weixia (Bonnie), Penumarthy, Shashikant & Börner, Katy. (2007). Designing Highly Flexible and Usable Cyberinfrastructures for Convergence. In Bainbridge, William S. & Roco, Mihail C. (Eds.), Progress in Convergence - Technologies for Human Wellbeing (Vol. 1093, pp. 161-179), Annals of the New York Academy of Sciences, Boston, MA.

Computational Proteomics

What relationships exist between protein targets of all drugs and all disease-gene products in the human protein–protein interaction network?

Yildriim, Muhammed A., Kwan-Il Goh, Michael E. Cusick, Albert-László Barabási, and Marc Vidal. (2007). Drug-target Network. Nature Biotechnology 25 no. 10: 1119-1126.

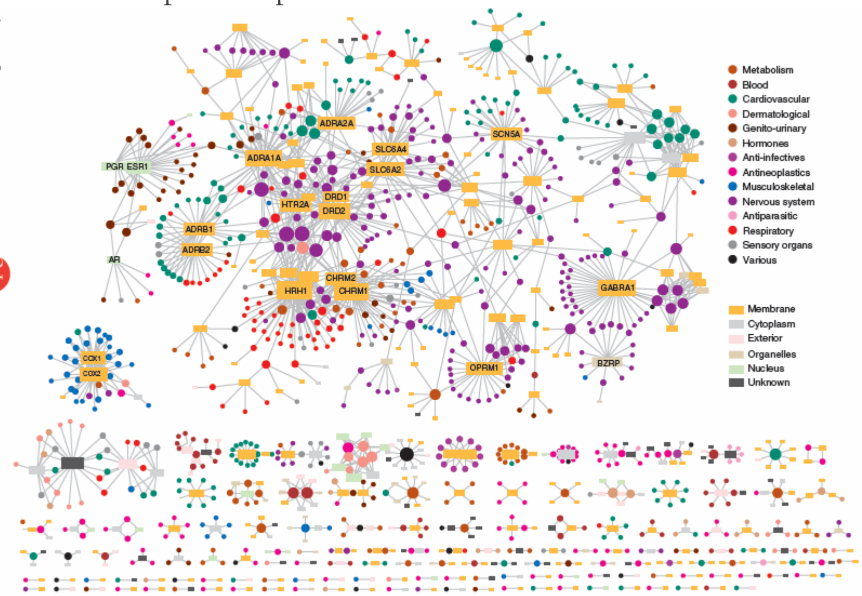


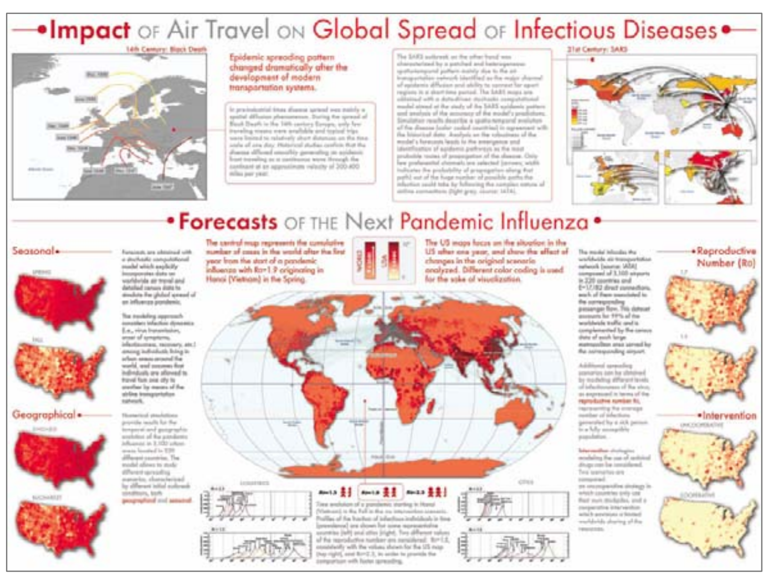
Figure 2 Drug–target network (DT network). The DT network is generated by using the known associations between FDA-approved drugs and their target proteins. Circles and rectangles correspond to drugs and target proteins, respectively. A link is placed between a drug node and a target node if the protein is a known target of that drug. The area of the drug (protein) node is proportional to the number of targets that the drug has (the number of drugs targeting the protein). Color codes are given in the legend. Drug nodes (circles) are colored according to their Anatomical Therapeutic Chemical Classification, and the target proteins (rectangular boxes) are colored according to their cellular component obtained from the Gene Ontology database.

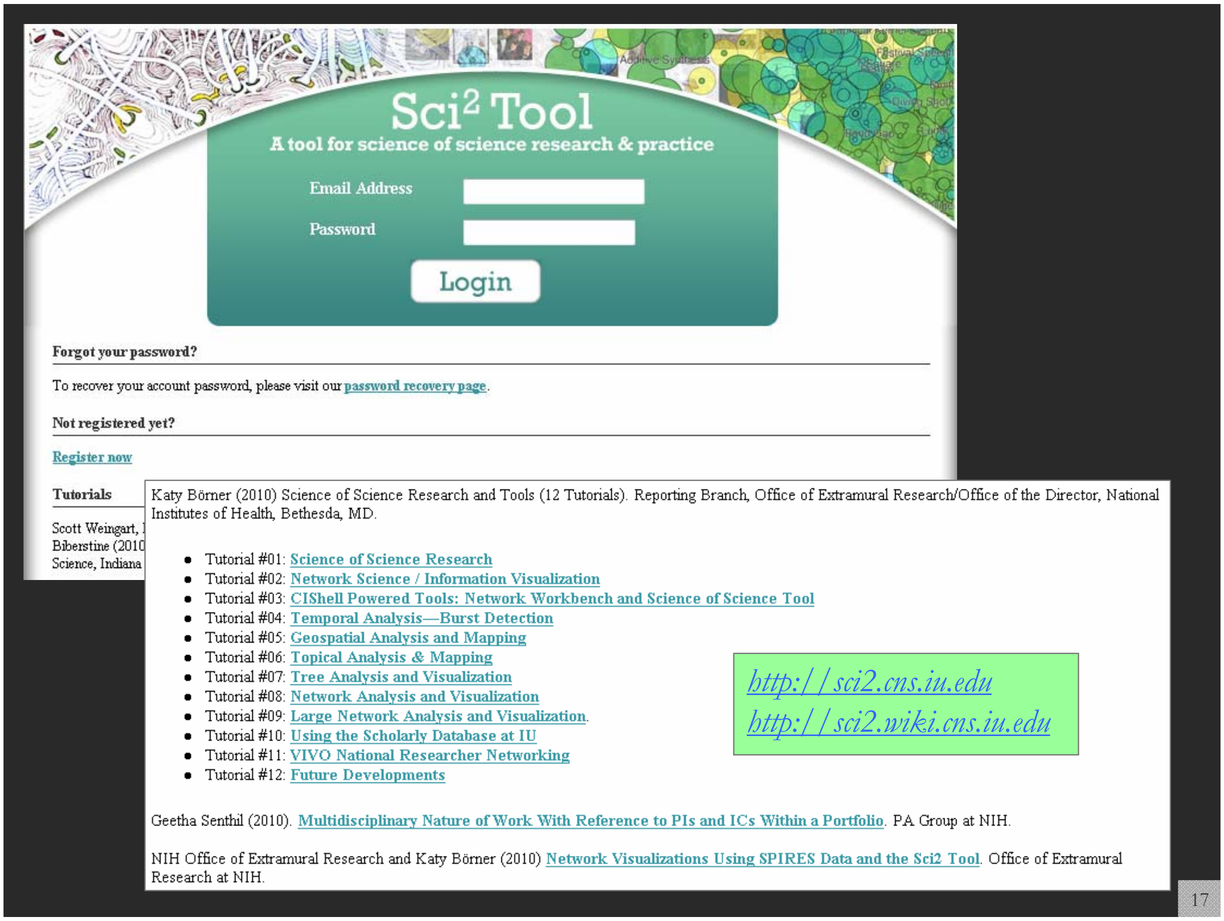
Computational Epidemics

Forecasting (and preventing the effects of) the next pandemic.

Epidemic Modeling in Complex realities, V. Colizza, A. Barrat, M. Barthelemy, A.Vespignani, Comptes Rendus Biologie, 330, 364-374 (2007).
Reaction-diffusion processes and metapopulation models in heterogeneous networks, V.Colizza, R. Pastor-Satorras, A.Vespignani, Nature Physics 3, 276-282 (2007).

Modeling the Worldwide Spread of Pandemic Influenza: Baseline Case and Containment Interventions, V. Colizza, A. Barrat, M. Barthelemy, A.-J. Valleron, A.Vespignani, PloS-Medicine 4, e13, 95-110 (2007).



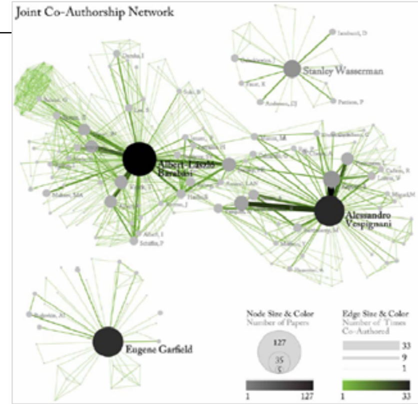


Type of Analysis vs. Level of Analysis

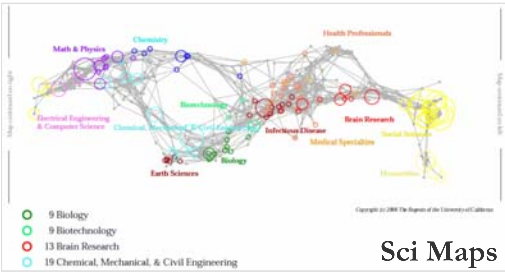
	Micro/Individual (1-100 records)	***Meso/Local (101–10,000 records)***	***Macro/Global (10,000 < records)***
Statistical Analysis/Profiling	Individual person and their expertise profiles	Larger labs, centers, universities, research domains, or states	All of NSF, all of USA, all of science.
Temporal Analysis (When)	Funding portfolio of one individual	Mapping topic bursts in 20-years of PNAS	113 Years of Physics Research
Geospatial Analysis (Where)	Career trajectory of one individual	Mapping a states intellectual landscape	PNAS Publications
Topical Analysis (What)	Base knowledge from which one grant draws.	Knowledge flows in Chemistry research	VxOrd/Topic maps of NIH funding
Network Analysis (With Whom?)	NSF Co-PI network of one individual	Co-author network	NSF's core competency

Sci² Tool – "Open Code for S&T Assessment"

OSGi/CIShell powered tool with NWB plugins and many new scientometrics and visualizations plugins.

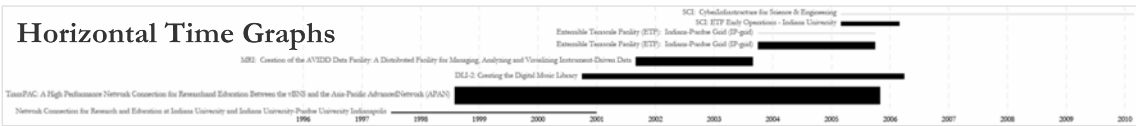


GUESS Network Vis



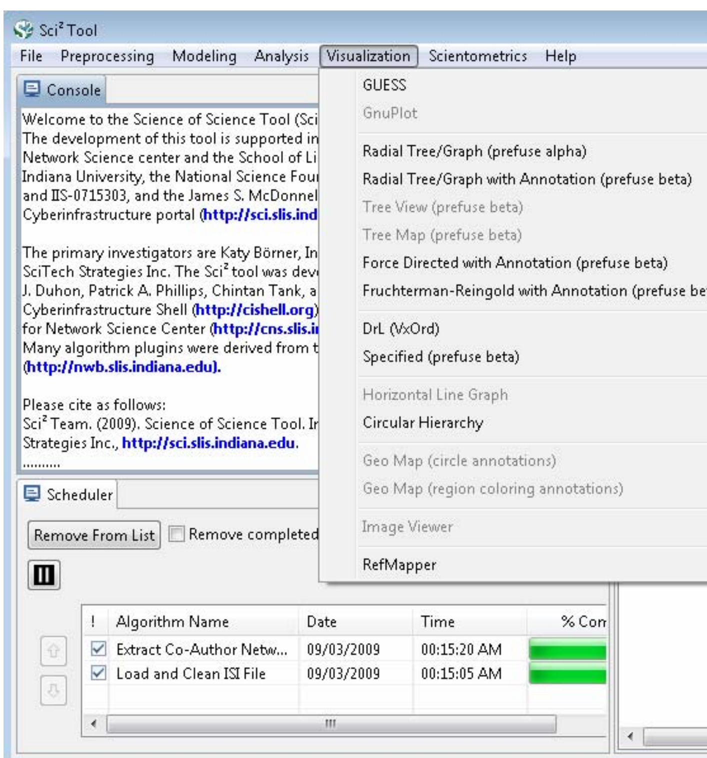
Sci Maps

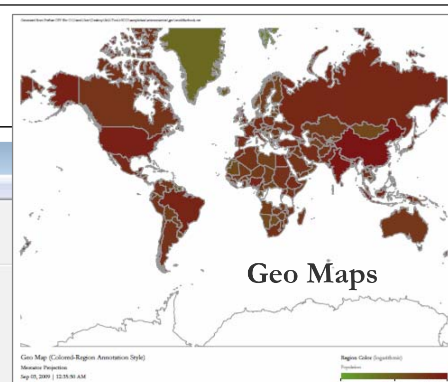
Horizontal Time Graphs



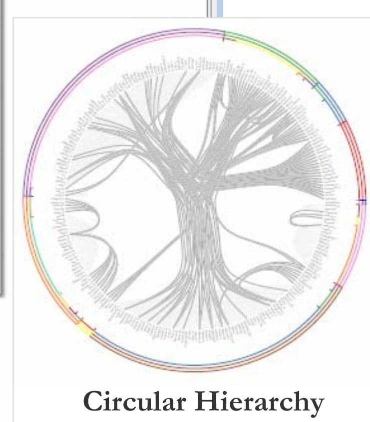
Börner, Katy, Huang, Weixia (Bonnie), Linnemeier, Micah, Duhon, Russell Jackson, Phillips, Patrick, Ma, Nianli, Zoss, Angela, Guo, Hanning & Price, Mark. (2009). Rete-Netzwerk-Red: Analyzing and Visualizing Scholarly Networks Using the Scholarly Database and the Network Workbench Tool. Proceedings of ISSI 2009: 12th International Conference on Scientometrics and Informetrics, Rio de Janeiro, Brazil, July 14-17 . Vol. 2, pp. 619-630.

Sci² Tool





Geo Maps



Circular Hierarchy

Sci² Tool: Algorithms

See https://nwb.slis.indiana.edu/community

Preprocessing
Extract Top N% Records
Extract Top N Records
Normalize Text
Slice Table by Line

Extract Top Nodes
Extract Nodes Above or Below Value
Delete Isolates

Extract top Edges
Extract Edges Above or Below Value
Remove Self Loops
Trim by Degree
MST-Pathfinder Network Scaling
Fast Pathfinder Network Scaling

Snowball Sampling (in nodes)
Node Sampling
Edge Sampling

Symmetrize
Dichotomize
Multipartite Joining

Geocoder

Extract ZIP Code

Modeling
Random Graph
Watts-Strogatz
Small World
Barabási-Albert Scale-Free
TARL

Analysis
Network Analysis Toolkit (NAT)
Unweighted & Undirected
    Node Degree
    Degree Distribution

    K-Nearest Neighbor (Java)
    Watts-Strogatz Clustering Coefficient
    Watts Strogatz Clustering Coefficient over K

    Diameter
    Average Shortest Path
    Shortest Path Distribution
    Node Betweenness Centrality

    Weak Component Clustering
    Global Connected Components

    Extract K-Core
    Annotate K-Coreness

    HITS

Weighted & Undirected
    Clustering Coefficient
    Nearest Neighbor Degree
    Strength vs Degree
    Degree & Strength
    Average Weight vs End-point Degree
    Strength Distribution
    Weight Distribution
    Randomize Weights

    Blondel Community Detection

    HITS
Unweighted & Directed
    Node Indegree
    Node Outdegree
    Indegree Distribution
    Outdegree Distribution

    K-Nearest Neighbor
    Single Node in-Out Degree Correlations

    Dyad Reciprocity
    Arc Reciprocity
    Adjacency Transitivity

    Weak Component Clustering
    Strong Component Clustering

Sci² Tool: Algorithms cont.

See https://nwb.slis.indiana.edu/community

    Extract K-Core
    Annotate K-Coreness

    HITS
    PageRank
Weighted & Directed
    HITS
    Weighted PageRank

Textual
Burst Detection

Visualization
GnuPlot
GUESS
Image Viewer

Radial Tree/Graph (prefuse alpha)
Radial Tree/Graph with Annotation
    (prefuse beta)
Tree View (prefuse beta)
Tree Map (prefuse beta)
Force Directed with Annotation
    (prefuse beta)
Fruchterman-Reingold with Annotation
    (prefuse beta)

DrL (VxOrd)
Specified (prefuse beta)

Horizontal Bar Graph
Circular Hierarchy
Geo Map (Circle Annotation Style)
Geo Map (Colored-Region Annotation Style)
Science Map (Circle Annotation)

Scientometrics
Remove ISI Duplicate Records
Remove Rows with Multitudinous Fields
Detect Duplicate Nodes
Update Network by Merging Nodes

Extract Directed Network
Extract Paper Citation Network
Extract Author Paper Network

Extract Co-Occurrence Network
Extract Word Co-Occurrence Network
Extract Co-Author Network
Extract Reference Co-Occurrence
    (Bibliographic Coupling) Network

Extract Document Co-Citation Network

Soon:
Database support for ISI and NSF data.

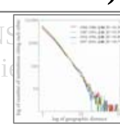
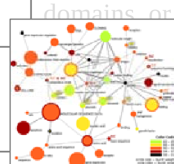
Contents

See Sci2 Tool Wiki
http://sci2.wiki.cns.iu.edu

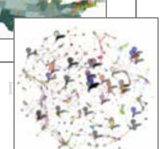
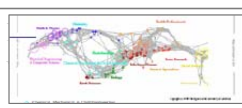
Sci2 A tool for science of science research & practice

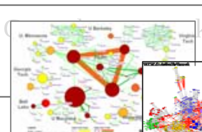
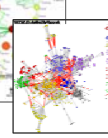
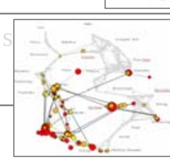
Type of Analysis vs. Level of Analysis

	Micro/Individual (1-100 records)	*Meso/Local (101–10,000 records)*	*Macro/Global (10,000 < records)*
Statistical Analysis/Profiling	Individual person and their expertise profiles	Larger labs, centers, universities, research domains, or states	All of NS SA, all of sci
Temporal Analysis (When)	Funding portfolio of one individual	ic bursts f PNAS	113 Years of P Research
Geospatial Analysis (Where)	Career trajectory of one individual	Mapping a s intellectual l	PNAS
Topical Analysis (What)	s.	flows in research	VxOrd/Topic NIH funding
Network Analysis (With Whom?)	NSF work of one	k	NIH's cy

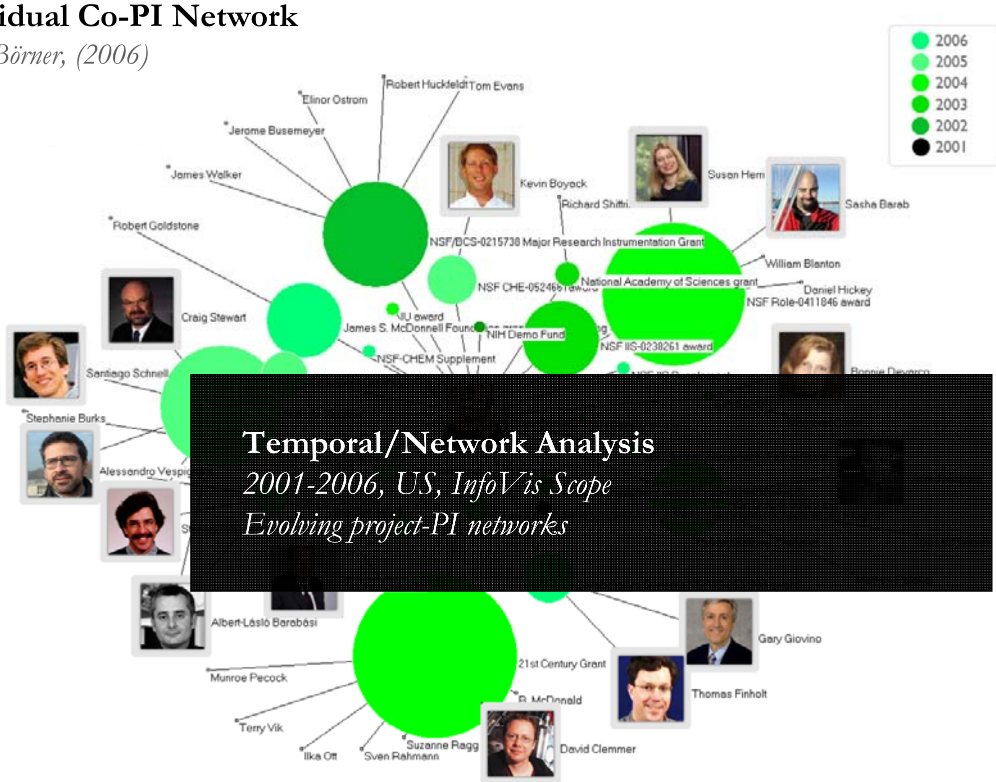


Individual Co-PI Network

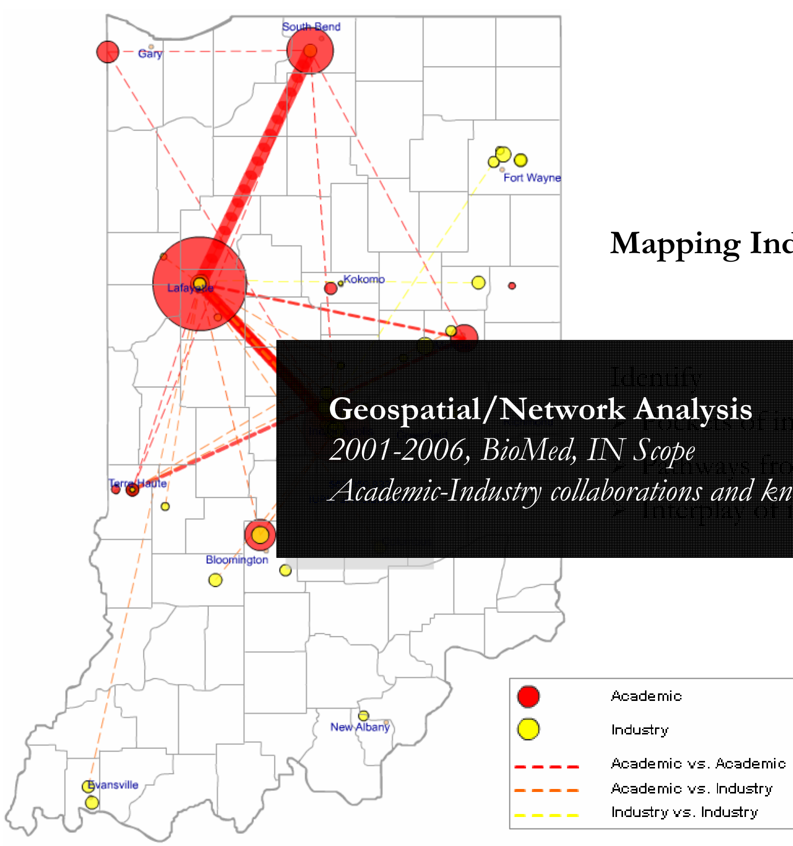
Ke & Börner, (2006)



Temporal/Network Analysis

2001-2006, US, InfoVis Scope

Evolving project-PI networks



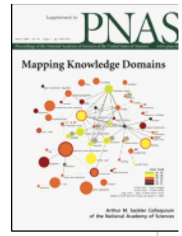
Mapping Indiana's Intellectual Space

Geospatial/Network Analysis

2001-2006, BioMed, IN Scope

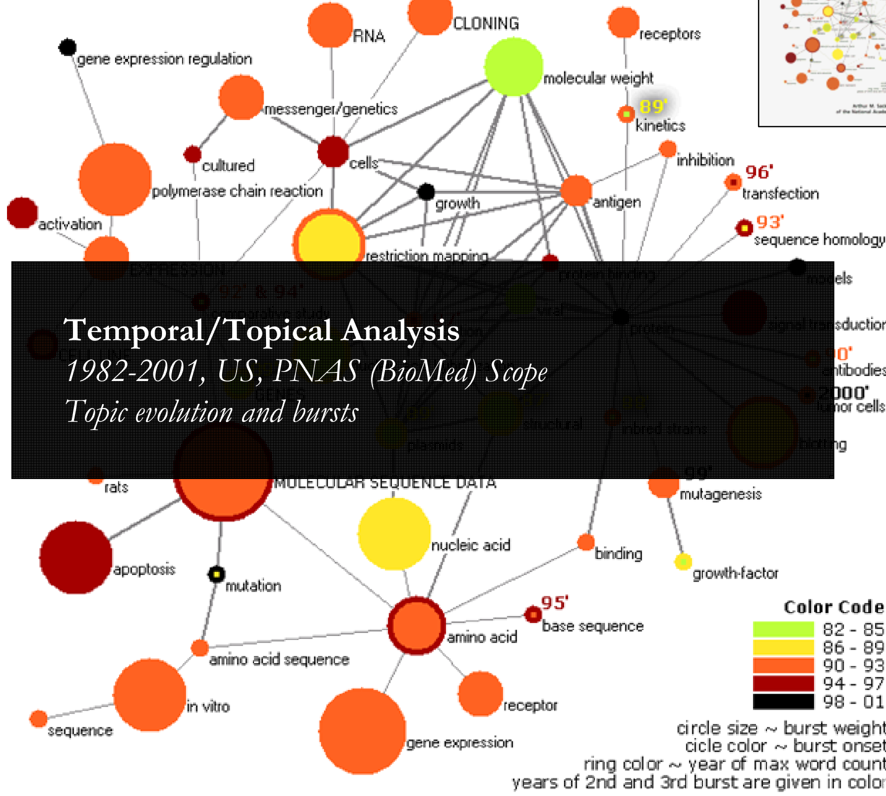
Academic-Industry collaborations and knowledge diffusion

Mapping Topic Bursts



Co-word space of the top 50 highly frequent and bursty words used in the top 10% most highly cited PNAS publications in 1982-2001.

Mane & Börner. (2004) PNAS, 101(Suppl. 1): 5287-5290.

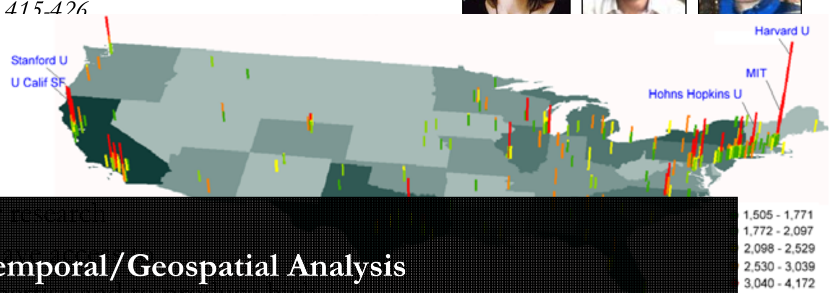


Temporal/Topical Analysis
1982-2001, US, PNAS (BioMed) Scope
Topic evolution and bursts

Spatio-Temporal Information Production and Consumption of Major U.S. Research Institutions

Börner, Katy, Penumarthy, Shashikant, Meiss, Mark and Ke, Weimao. (2006) Mapping the Diffusion of Scholarly Knowledge Among Major U.S. Research Institutions. Scientometrics. 68(3), pp. 415-426.





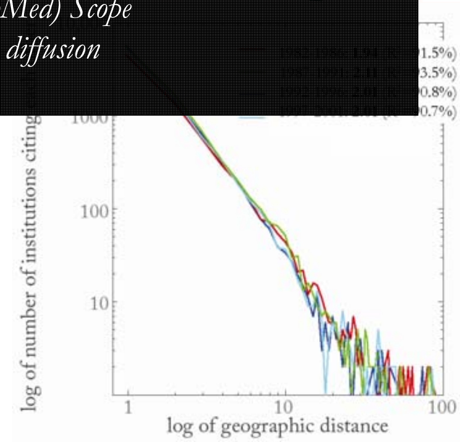
Research questions:

1. Does space still matter in the Internet age?
2. Does one still have to study and work at major research institutions in order to have access to high quality data and [illegible] quality research?
3. Does the Internet lead to more global citation patterns, i.e., more citation links between papers produced at geographically distant research instructions?

Temporal/Geospatial Analysis
1982-2001, US, PNAS (BioMed) Scope
Citation impact and knowledge diffusion

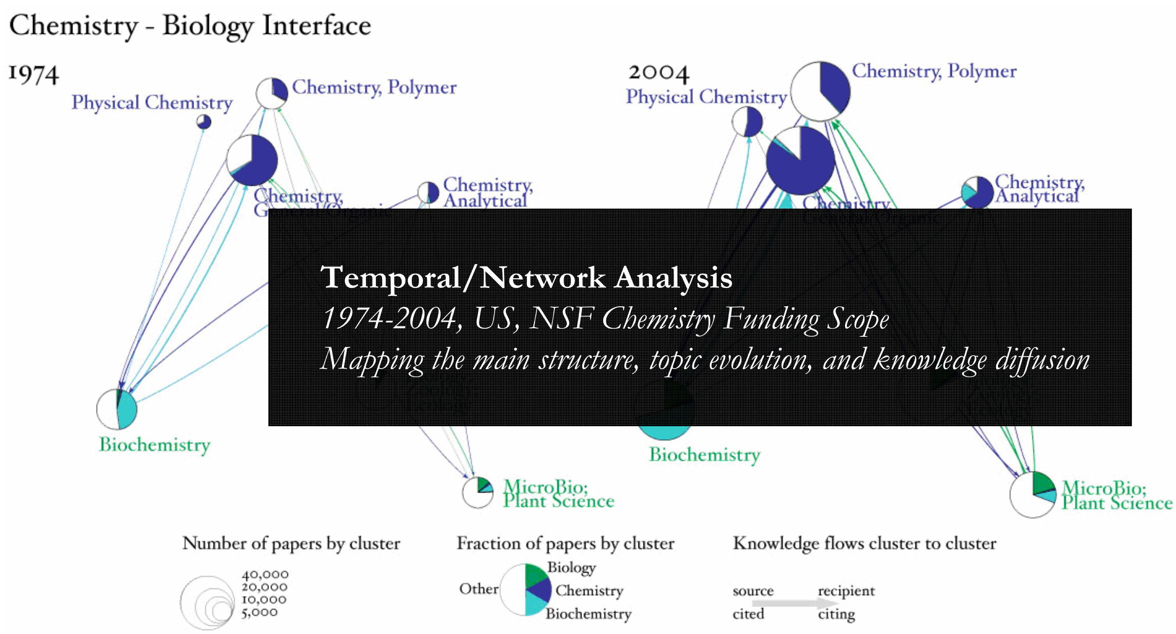
Contributions:

- Answer to Qs 1 + 2 is YES.
- Answer to Qs 3 is NO.
- Novel approach to analyzing the dual role of institutions as information producers and consumers and to study and visualize the diffusion of information among them.



Topical Composition and Knowledge Flow Patterns in Chemistry Research for 1974 and 2004

Kevin W. Boyack, Katy Börner, & Richard Klavans (2007)



Temporal/Network Analysis

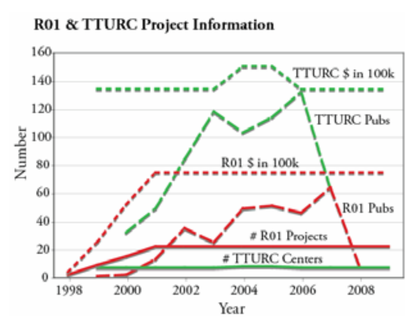
1974-2004, US, NSF Chemistry Funding Scope

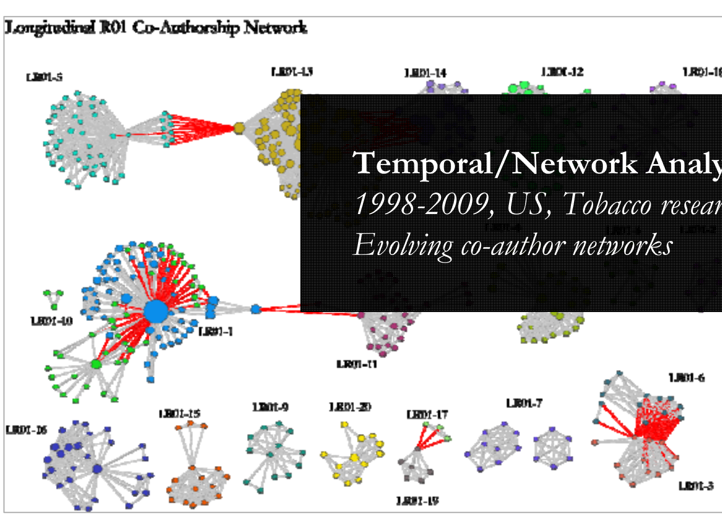
Mapping the main structure, topic evolution, and knowledge diffusion

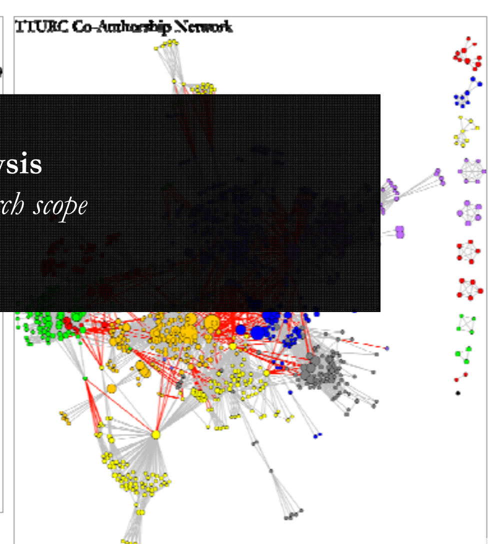
Mapping Transdisciplinary Tobacco Use Research Centers Publications

Compare R01 investigator based funding with TTURC Center awards in terms of number of publications and evolving co-author networks.

Zoss & Börner, forthcoming.







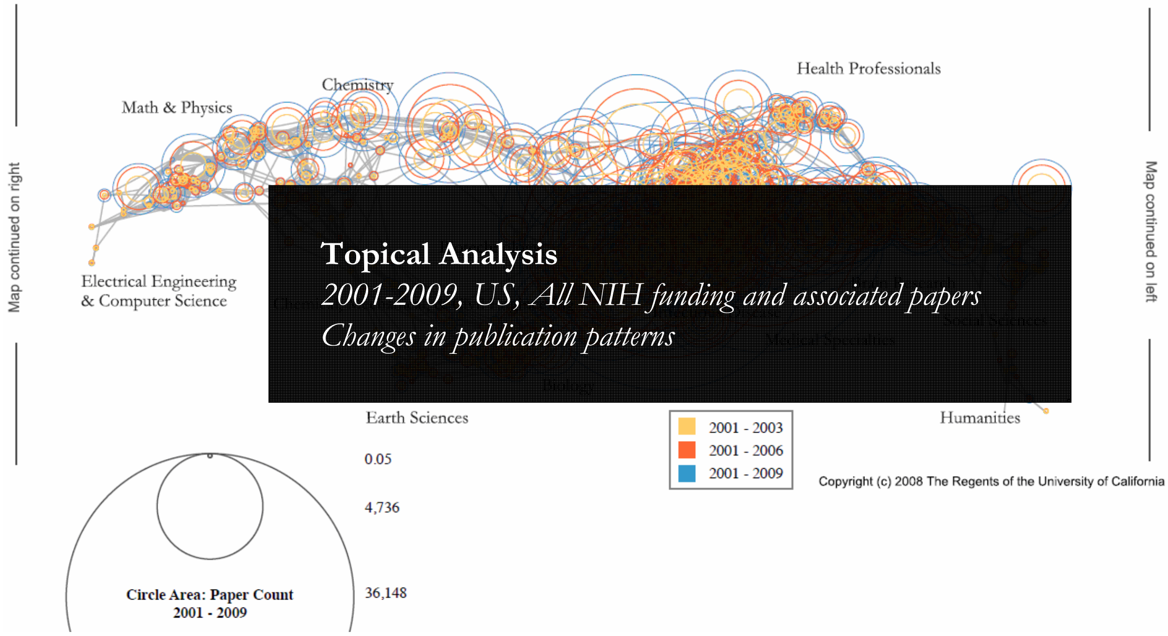
Temporal/Network Analysis

1998-2009, US, Tobacco research scope

Evolving co-author networks

MEDLINE Publication Output by The National Institutes of Health (NIH) Using Nine Years of ExPORTER Data

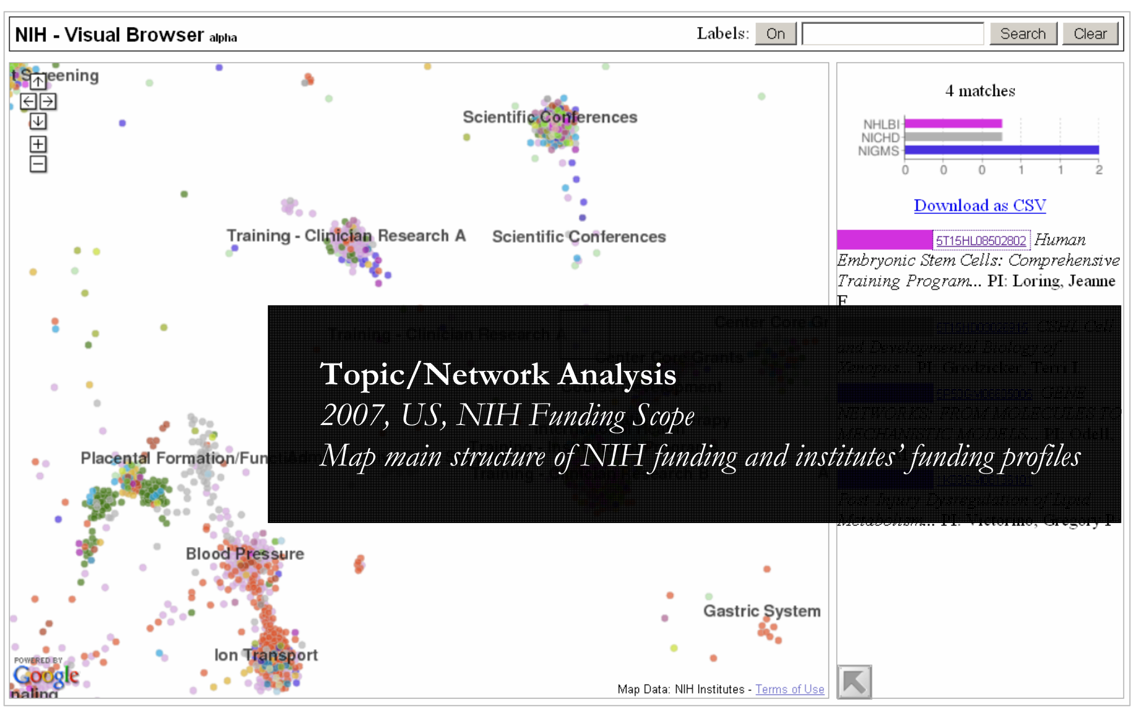
Katy Börner, Nianli Ma, Joseph R. Biberstine, Cyberinfrastructure for Network Science Center, SLIS, Indiana University, Robin M. Wagner, Rediet Berhane, Hong Jiang, Susan E. Ivey, Katrina Pearson and Carl McCabe, Reporting Branch, Division of Information Services, Office of Research Information Systems, Office of Extramural Research, Office of the Director, National Institutes of Health (NIH), Bethesda, MD.



Topical Analysis
2001-2009, US, All NIH funding and associated papers
Changes in publication patterns

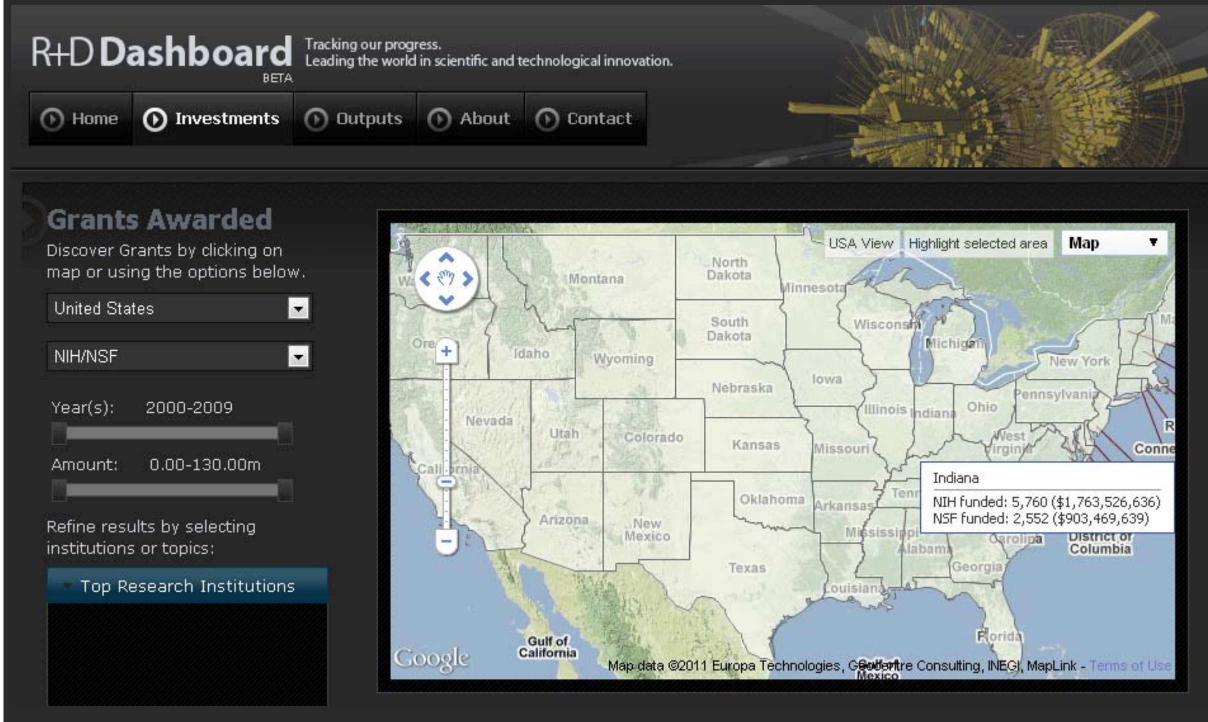
Interactive Science Map of NIH Funding

Herr II, Bruce W., Talley, Edmund M, Burns, Gully APC, Newman, David & La Rowe, Gavin. (2009).



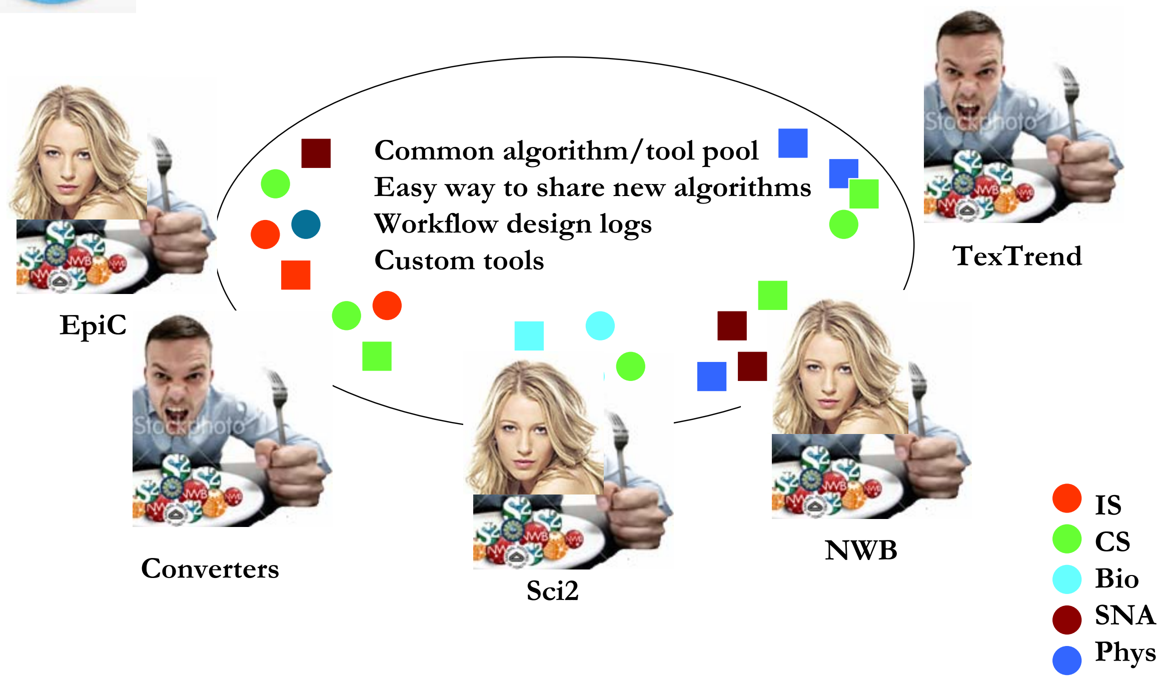
Topic/Network Analysis
2007, US, NIH Funding Scope
Map main structure of NIH funding and institutes' funding profiles

http://scimaps.org/maps/nih/2007



http://rd-dashboard.nitrd.gov

Changing Scientific Landscape—Personal Observations Cont.



OSGi/CIShell Adoption

CIShell/OSGi is at the core of different CIs and a total of 169 unique plugins are used in the

- ***Information Visualization*** (http://iv.slis.indiana.edu),
- ***Network Science (NWB Tool)*** (http://nwb.slis.indiana.edu),
- ***Scientometrics and Science Policy (Sci^2 Tool)*** (http://sci.slis.indiana.edu), and
- ***Epidemics*** (http://epic.slis.indiana.edu) research communities.

Most interestingly, a number of other projects recently adopted OSGi and one adopted CIShell:

Cytoscape (http://www.cytoscape.org) lead by Trey Ideker, UCSD is an open source bioinformatics software platform for visualizing molecular interaction networks and integrating these interactions with gene expression profiles and other state data (Shannon et al., 2002).

Taverna Workbench (http://taverna.sourceforge.net) lead by Carol Goble, University of Manchester, UK is a free software tool for designing and executing workflows (Hull et al., 2006). Taverna allows users to integrate many different software tools, including over 30,000 web services.

MAEviz (https://wiki.ncsa.uiuc.edu/display/MAE/Home) managed by Shawn Hampton, NCSA is an open-source, extensible software platform which supports seismic risk assessment based on the Mid-America Earthquake (MAE) Center research.

TEXTrend (http://www.textrend.org) lead by George Kampis, Eötvös University, Hungary develops a framework for the easy and flexible integration, configuration, and extension of plugin-based components in support of natural language processing (NLP), classification/mining, and graph algorithms for the analysis of business and governmental text corpuses with an inherently temporal component.

As the functionality of OSGi-based software frameworks improves and the number and diversity of dataset and algorithm plugins increases, the capabilities of custom tools will expand.

Acknowledgements

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- Software development benefits greatly from the open-source community. Full software credits are distributed with the source, but I would especially like to acknowledge Jython, JUNG, Prefuse, GUESS, GnuPlot, and OSGi, as well as Apache Derby, used in the Sci2 tool.

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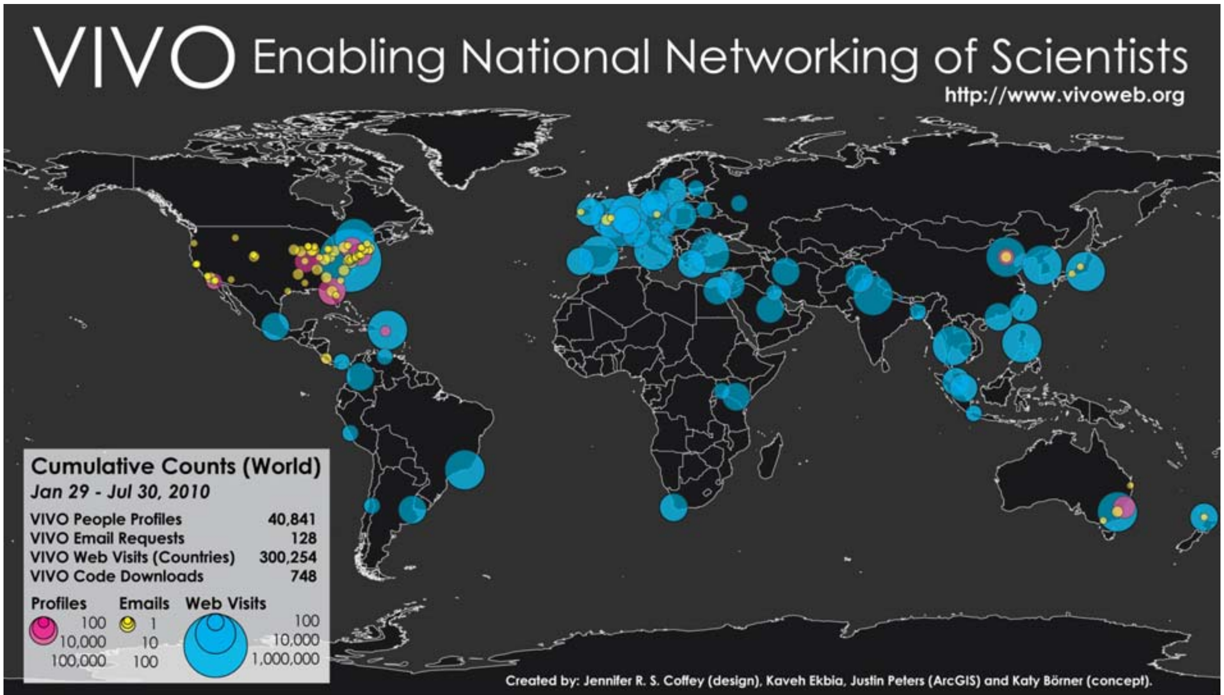
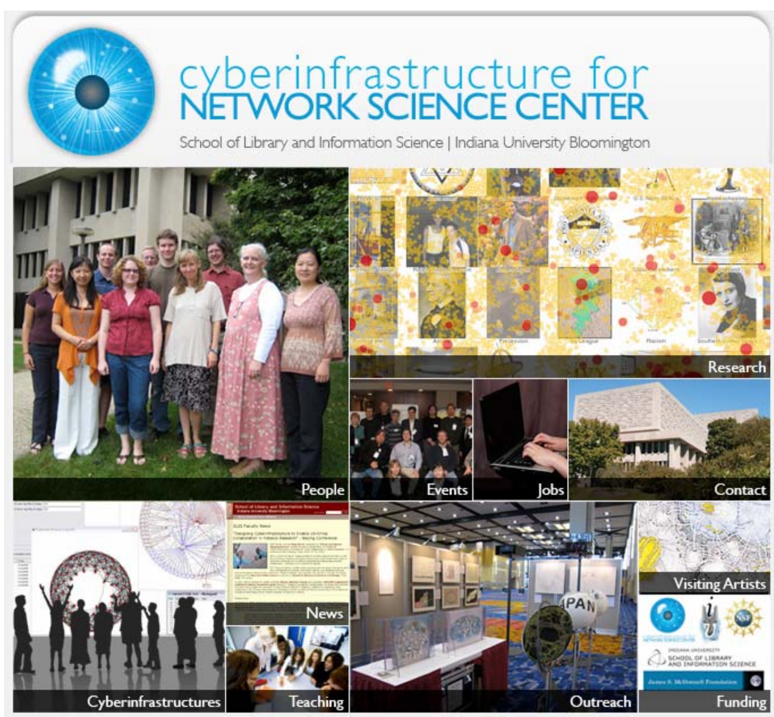


VIVO 1.0 source code was publicly released on April 14, 2010
87 downloads by June 11, 2010.
The more institutions adopt VIVO, the more high quality data will be available to understand, navigate, manage, utilize, and communicate progress in science and technology.



All papers, maps, cyberinfrastructures, talks, press are linked from http://cns.slis.indiana.edu