# Towards Plug-and-Play Macroscopes for Science Policy Decision Making

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With special thanks to the members at the Cyberinfrastructure for Network Science Center and the Mapping Science exhibit map makers and advisory board members.

JST-CRDS Workshop Evidence-based Policy Making for Science, Technology and Innovation Policy Center for Research and Development Strategy (CRDS), Tokyo, Japan

March 9-10, 2010





# The Need.

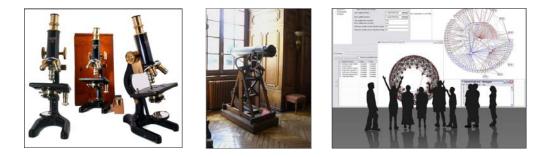


# The Changing Scientific Landscape

- Star Scientist -> Research Teams: In former times, science was driven by key scientists. Today, science is driven by effectively collaborating co-author teams often comprising expertise from multiple disciplines and several geospatial locations (Börner, Dall'Asta, Ke, & Vespignani, 2005; Shneiderman, 2008).
- *Users -> Contributors:* Web 2.0 technologies empower anybody to contribute to Wikipedia and to exchange images and videos via Fickr and YouTube. WikiSpecies, WikiProfessionals, or WikiProteins combine wiki and semantic technology in support of real time community annotation of scientific datasets (Mons et al., 2008).
- *Cross-disciplinary:* The best tools frequently borrow and synergistically combine methods and techniques from different disciplines of science and empower interdisciplinary and/or international teams of researchers, practitioners, or educators to fine-tune and interpret results collectively.
- **One Specimen -> Data Streams:** Microscopes and telescopes were originally used to study one specimen at a time. Today, many researchers must make sense of massive streams of multiple types of data with different formats, dynamics, and origin.
- Static Instrument -> Evolving Cyberinfrastructure (CI): The importance of hardware instruments that are rather static and expensive decreases relative to software infrastructures that are highly flexible and continuously evolving according to the needs of different sciences. Some of the most successful services and tools are decentralized increasing scalability and fault tolerance.
- **Modularity:** The design of software modules with well defined functionality that can be flexibly combined helps reduce costs, makes it possible to have many contribute, and increases flexibility in tool development, augmentation, and customization.
- **Standardization:** Adoption of standards speeds up development as existing code can be leveraged. It helps pool resources, supports interoperability, but also eases the migration from research code to production code and hence the transfer of research results into industry applications and products.
- *Open data and open code:* Lets anybody check, improve, or repurpose code and eases the replication of scientific studies.



Microscopes, Telescopes, and Macrocopes



Just as the **microscope** empowered our naked eyes to see cells, microbes, and viruses thereby advancing the progress of biology and medicine or the **telescope** opened our minds to the immensity of the cosmos and has prepared mankind for the conquest of space, **macroscopes** promise to help us cope with another infinite: the infinitely complex. Macroscopes give us a 'vision of the whole' and help us 'synthesize'. They let us detect patterns, trends, outliers, and access details in the landscape of science. Instead of making things larger or smaller, macroscopes let us observe what is at once too great, too slow, or too complex for our eyes.



# **Desirable Features of Plug-and-Play Macroscopes**

- *Division of Labor:* Ideally, labor is divided in a way that the expertise and skills of computer scientists are utilized for the design of standardized, modular, easy to maintain and extend "core architecture". Dataset and algorithm plugins, i.e., the "filling", are initially provided by those that care and know most about the data and developed the algorithms: the domain experts.
- *Ease of Use:* As most plugin contributions and usage will come from non-computer scientists it must be possible to contribute, share, and use new plugins without writing one line of code. Wizard-driven integration of new algorithms and data sets by domain experts, sharing via email or online sites, deploying plugins by adding them to the 'plugin' directory, and running them via a Menu driven user interfaces (as used in Word processing systems or Web browsers) seems to work well.
- **Plugin Content and Interfaces:** Should a plugin represent one algorithm or an entire tool? What about data converters needed to make the output of one algorithm compatible with the input of the next? Should those be part of the algorithm plugin or should they be packaged separately?
- **Supported (Central) Data Models:** Some tools use a central data model to which all algorithms conform, e.g., Cytoscape, see Related Work section. Other tools support many internal data models and provide an extensive set of data converters, e.g., Network Workbench, see below. The former often speeds up execution and visual rendering while the latter eases the integration of new algorithms. In addition, most tools support an extensive set of input and output formats.
- *Core vs. Plugins:* As will be shown, the "core architecture" and the "plugin filling" can be implemented as sets of plugin bundles. Answers to questions such as: "Should the graphical user interface (GUI), interface menu, scheduler, or data manager be part of the core or its filling?" will depend on the type of tools and services to be delivered.
- **Supported Platforms:** If the software is to be used via Web interfaces then Web services need to be implemented. If a majority of domain experts prefers a stand-alone tool running on a specific operating system then a different deployment is necessary.

# A Solution.



CI for a Science of Science Studies

**NST** 

Scholarly Database: 23 million scholarly records <u>http://sdb.slis.indiana.edu</u>

James S. McDonnell Foundation



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



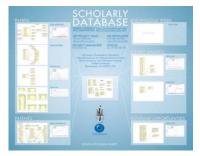
Network Workbench Tool + Community Wiki http://nwb.slis.indiana.edu

<u>ss</u>

Sci<sup>2</sup> Tool and Science of Science CI Portal http://sci.slis.indiana.edu



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





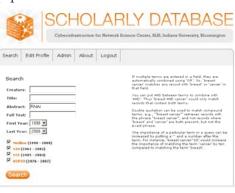
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Scholarly Database: Web Interface

Search across publications, patents, grants.

Download records and/or (evolving) co-author, paper-citation networks.

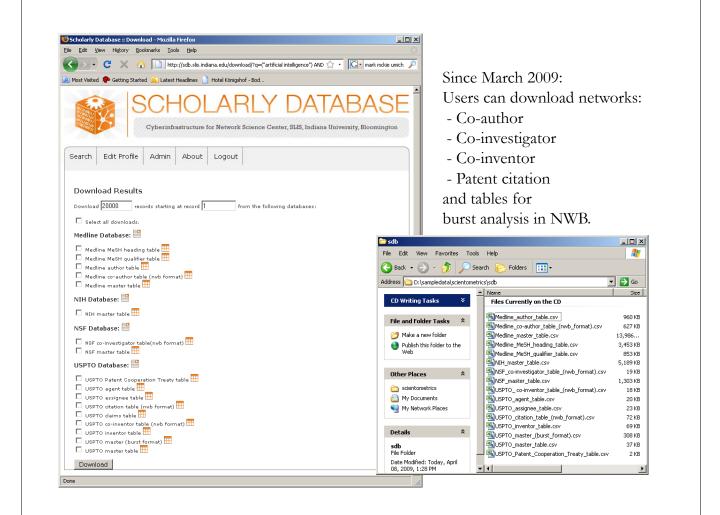
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Register for free access at http://sdb.slis.indiana.edu

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# Scholarly Database: # Records, Years Covered

Dataset	# Records	Years Covered	Updated	Restricted Access
Medline	17,764,826	1898-2008	Yes	
PhysRev	398,005	1893-2006		Yes
PNAS	16,167	1997-2002		Yes
JCR	59,078	1974, 1979, 1984, 1989 1994-2004		Yes
USPTO	3, 875,694	1976-2008	Yes*	
NSF	174,835	1985-2002	Yes*	
NIH	1,043,804	1961-2002	Yes*	
Total	23,167,642	1893-2006	4	3

Datasets available via the Scholarly Database (\* internally)

Aim for comprehensive time, geospatial, and topic coverage.

# NetworkWorkbench

Network Workbench Tool

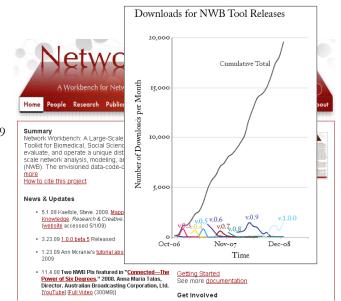


The Network Workbench (NWB) tool supports researchers, educators, and practitioners interested in the study of biomedical, social and behavioral science, physics, and other networks.

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 35,000 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.

Networkworkbench NWB Tool Interface Components 🐵 Network Workbench Tool File Preprocessing Modeling Analysis Visualization Scientometrics Help 🖵 🗖 🔢 Data Manager Console displays data operations (save, load, view, etc.) and algorithm input parameters, selection, & acknowledgements as well as error reporting. 🚍 Console 🛛 🔸 - -Welcome to the Netwo preprocessing, modeling, analysis, and ~ visualization of small, n The Network Workben is supported in part by the NSF Data Manager keeps track of all datasets that are available IIS-0513650 award. The primary investigators are or , kacy borner, Dr. Albert-László Barabási, Dr. Santiago Schnell, Dr. Alessandro Vespignani, Dr. Stanley Wasserman, and Dr. Eric A. Wernert. for algorithmic visualization or manipulation. The NWB tool was developed by Weixia Huang, Russell Duhon, Micah Linnemeier, Timothy Kelley, Duygu Balcan, Mariano Beiró, Bruce Herr, Santo Fortunato, Ben Markines, Felix Terkhorn, Heng Zhang, Megha Ramawat, César Hidalgo, Ramya Sabbineni, Vivek Thaires, Soma Sanyal, Ann McCranie, Alessandro Vespignani, and Katy Börner. It uses the Cyberinfrastructure Shell.org) developed at the Cyberinfrastructure for Network Science Center (http://cns.slis.indiana.edu) at Indiana University.

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Please cite as follows: NWB Team. (2006). Network Workbench Tool. Indiana University and Northeastern University, http://nwb.slis.indiana.edu

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Algorithm Name

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# NetworkWorkbench Project Details

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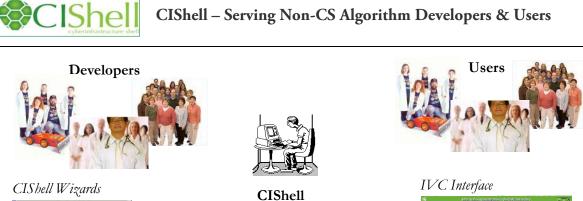
Investigators:	Katy Börner, Albert-Laszlo Barabasi, Santiago Schnell, Alessandro Vespignani & Stanley Wasserman, Eric Wernert
Software Team:	Lead: Micah Linnemeier
	Members: Patrick Phillips, Russell Duhon, Tim Kelley & Ann McCranie
	Previous Developers: Weixia (Bonnie) Huang, Bruce Herr, Heng Zhang, Duygu Balcan, Bryan Hook, Ben Markines, Santo Fortunato, Felix Terkhorn, Ramya Sabbineni, Vivek S. Thakre & Cesar Hidalgo
Goal:	Develop a large-scale network analysis, modeling and visualization toolkit for physics, biomedical, and social science research.
Amount:	\$1,120,926, NSF IIS-0513650 award
Duration:	Sept. 2005 - Aug. 2009
Website:	http://nwb.slis.indiana.edu

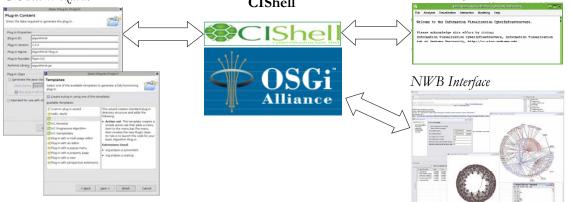


### **NWB** Advisory Board:

James Hendler (Semantic Web) <u>http://www.cs.umd.edu/~hendler/</u> Jason Leigh (CI) <u>http://www.evl.uic.edu/spiff/</u> Neo Martinez (Biology) <u>http://online.sfsu.edu/~webhead/</u> Michael Macy, Cornell University (Sociology) <u>http://www.soc.cornell.edu/faculty/macy.shtml</u> Ulrik Brandes (Graph Theory) <u>http://www.inf.uni-konstanz.de/~brandes/</u> Mark Gerstein, Yale University (Bioinformatics) <u>http://bioinfo.mbb.yale.edu/</u> Stephen North (AT&T) <u>http://public.research.att.com/viewPage.cfm?PageID=81</u> Tom Snijders, University of Groningen <u>http://stat.gamma.rug.nl/snijders/</u> Noshir Contractor, Northwestern University <u>http://www.spcomm.uiuc.edu/nosh/</u>









CIShell is built upon the Open Services Gateway Initiative (OSGi) Framework.

## OSGi (http://www.osgi.org) is

- A standardized, component oriented, computing environment for networked services.
- Successfully used in the industry from high-end servers to embedded mobile devices  $\geq$ since 8 years.
- $\geq$ Alliance members include IBM (Eclipse), Sun, Intel, Oracle, Motorola, NEC and many others.
- Widely adopted in open source realm, especially since Eclipse 3.0 that uses OSGi R4  $\geq$ for its plugin model.

### Advantages of Using OSGi

- Any CIShell algorithm is a service that can be used in any OSGi-framework based  $\geq$ system.
- Using OSGi, running CIShells/tools can connected via RPC/RMI supporting peer-to- $\geq$ peer sharing of data, algorithms, and computing power.

Ideally, CIShell becomes a standard for creating OSGi Services for algorithms.

# NetworkWorkbench NWB Tool: Supported Data Formats

#### Personal Bibliographies

- Bibtex (.bib)  $\geq$
- $\triangleright$ Endnote Export Format (.enw)

#### **Data Providers**

- Web of Science by Thomson Scientific/Reuters (.isi)
- Scopus by Elsevier (.scopus)
- ≻ Google Scholar (access via Publish or Perish save as CSV, Bibtex, EndNote)
- ≻ Awards Search by National Science Foundation (.nsf)

#### *Scholarly Database* (all text files are saved as .csv)

- Medline publications by National Library of Medicine
- $\geq$ NIH funding awards by the National Institutes of Health (NIH)
- $\geq$ NSF funding awards by the National Science Foundation (NSF)
- U.S. patents by the United States Patent and Trademark Office  $\triangleright$ (USPTO)
- Medline papers NIH Funding ≻

#### **Network Formats**

- NWB (.nwb)
- Pajek (.net)
- GraphML (.xml or .graphml)
- XGMML (.xml)

#### **Burst Analysis Format**

Burst (.burst)

#### **Other Formats**

- CSV (.csv)
- Edgelist (.edge)
- Pajek (.mat)
- TreeML (.xml)  $\geq$

Networkworkbench NWB Tool: Output Formats

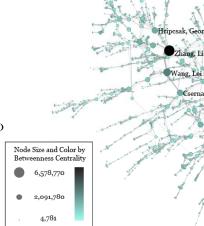
> NWB tool can be used for data conversion. Supported output formats comprise:

Medline Co-authorship Network Largest Component

- ► CSV (.csv)
- ► NWB (.nwb)
- Pajek (.net)  $\geq$
- ➢ Pajek (.mat)
- ➢ GraphML (.xml or .graphml)
- ► XGMML (.xml)
- ➢ GUESS

Supports export of images into common image file formats.

 Horizontal Bar Graphs saves out raster and ps files.



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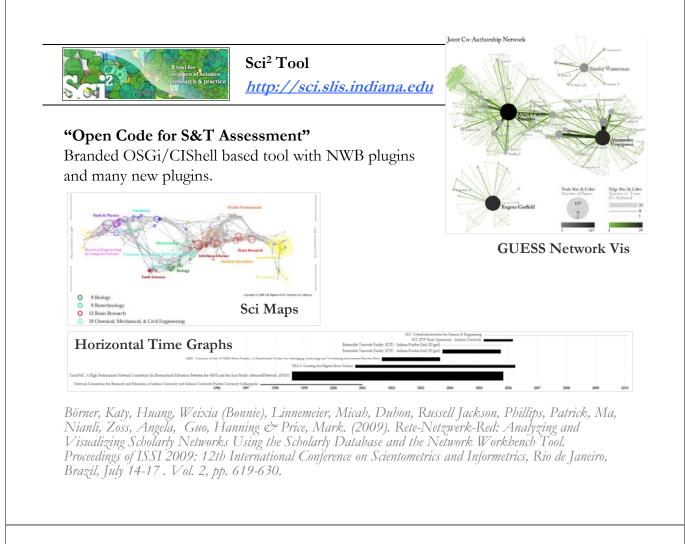
# Sci<sup>2</sup> Tool for Science of Science **Research and Practice**

File Preprocessing Modeling Analy	sis Visualizatio	n Sciento	metrics Help	
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#### Acknowledgments

This work is supported in part by the Cyberinfrastructure for Network Science center and the School of Library and Information Science at Indiana University, the National Science Foundation under Grant No. SBE-0738111 and IIS-0513650, and the James S. McDonnell Foundation.





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# Sci<sup>2</sup> Tool: Algorithms

See <u>https://nwb.slis.indiana.edu/community</u>

#### 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

23



Extract K-Core Annotate K-Coreness

HITS PageRank Weighted & Directed HITS Weighted PageRank

Textual Burst Detection

# Sci<sup>2</sup> Tool: Algorithms cont. See https://nwb.slis.indiana.edu/community

#### 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 Line Graph Circular Hierarchy Geo Map (Circle Annotation Style) Geo Map (Colored-Region Annotation Style) \*Science Map (Circle Annotation)

\* Requires permission from UCSD All four+ save into Postscript files.

#### **Scientometrics**

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

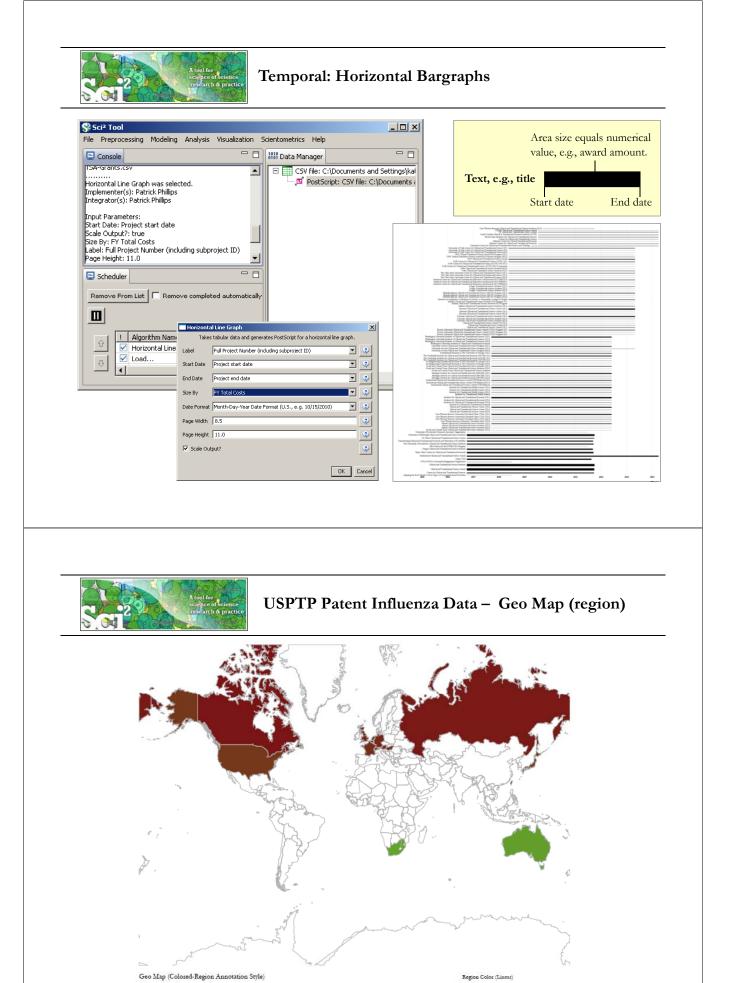
Extract Directed Network Extract Paper Citation Network Extract Author Paper Network

#### Extract Co-Occurrence Network

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

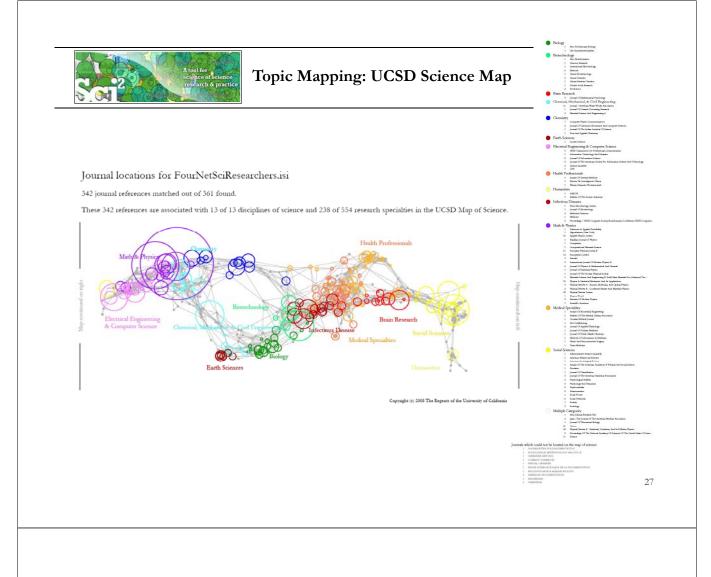
Extract Document Co-Citation Network

**General Network extraction** 



Mercator Projection Oct 19, 2009 | 09:28:22 PM Katy Borner

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# OSGi/CIShell Adoption

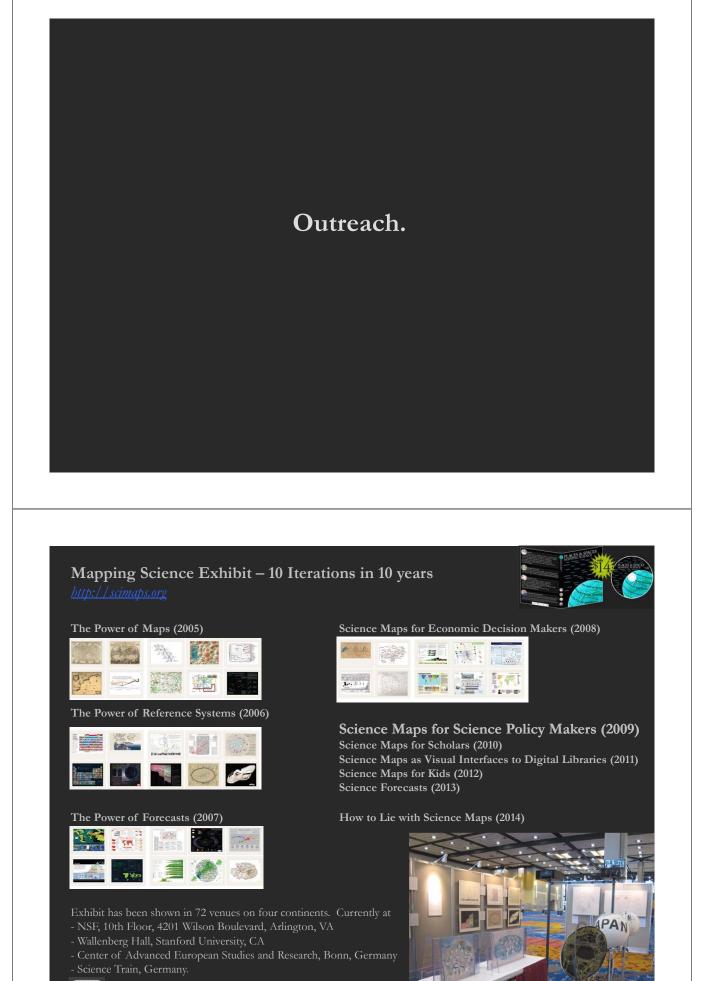
CIShell/OSGi is at the core of different CIs and a total of 169 unique plugins are used in the

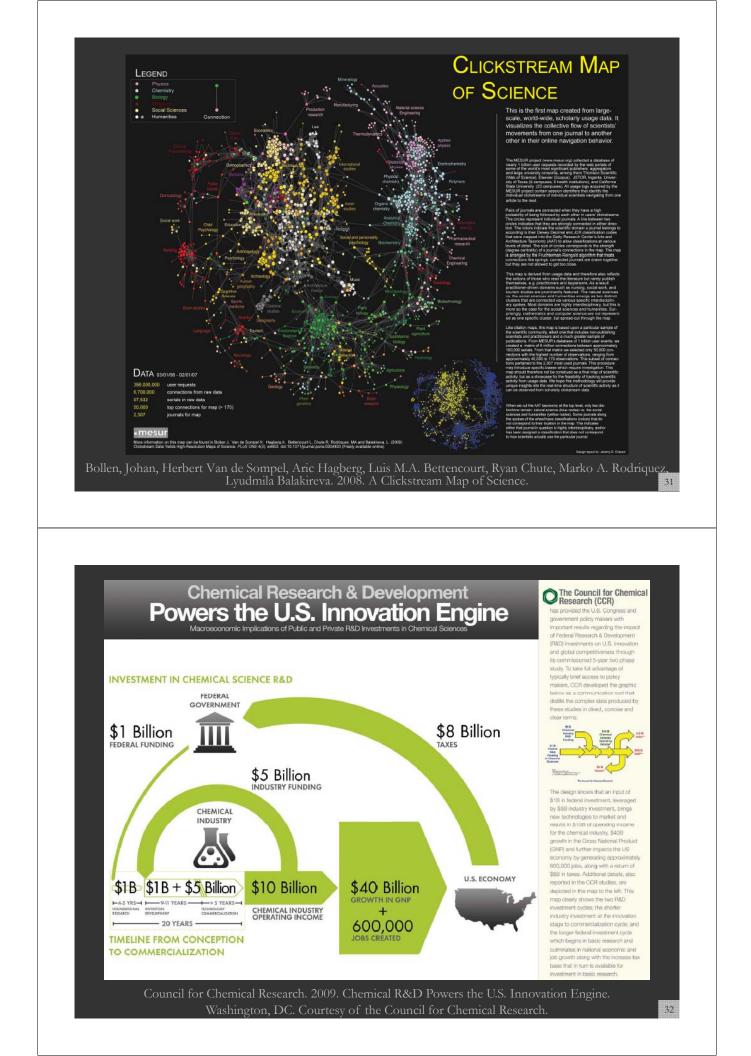
- Information Visualization (http://iv.slis.indiana.edu),
- Network Science (NWB Tool) (http://nwb.slis.indiana.edu),
- Scientometrics and Science Policy (Sci<sup>2</sup> Tool) (http://sci.slis.indiana.edu), and
- Epidemics (http://epic.slis.indiana.edu) research communities.

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

- *Cytoscape* (<u>http://www.cytoscape.org</u>) 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* (<u>http://taverna.sourceforge.net</u>) 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.





## **Illuminated Diagram Display**

W. Bradford Paley, Kevin W. Boyack, Richard Kalvans, and Katy Börner (2007) Mapping, Illuminating, and Interacting with Science. SIGGRAPH 2007.

## **Questions:**

- Who is doing research on what topic and where?
- What is the 'footprint' of interdisciplinary research fields?
- What impact have scientists?

## **Contributions:**

• Interactive, high resolution interface to access and make sense of data about scholarly activity.

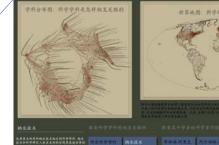






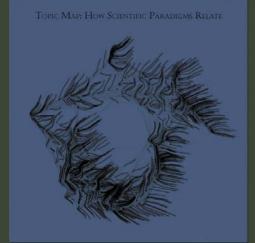
Large-scale, high resolution prints illuminated via projector or screen.

Interactive touch panel.





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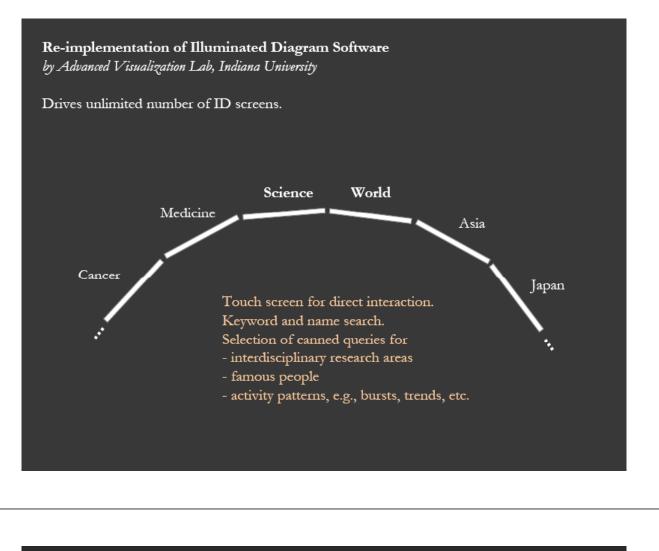


You may run your finger over each of these maps to control the lighting on the other: touching a place on the world map will light up topics studied in that place; touching a paradigm on the topic map will light up the places that study that topic.

#### Nanotechnology

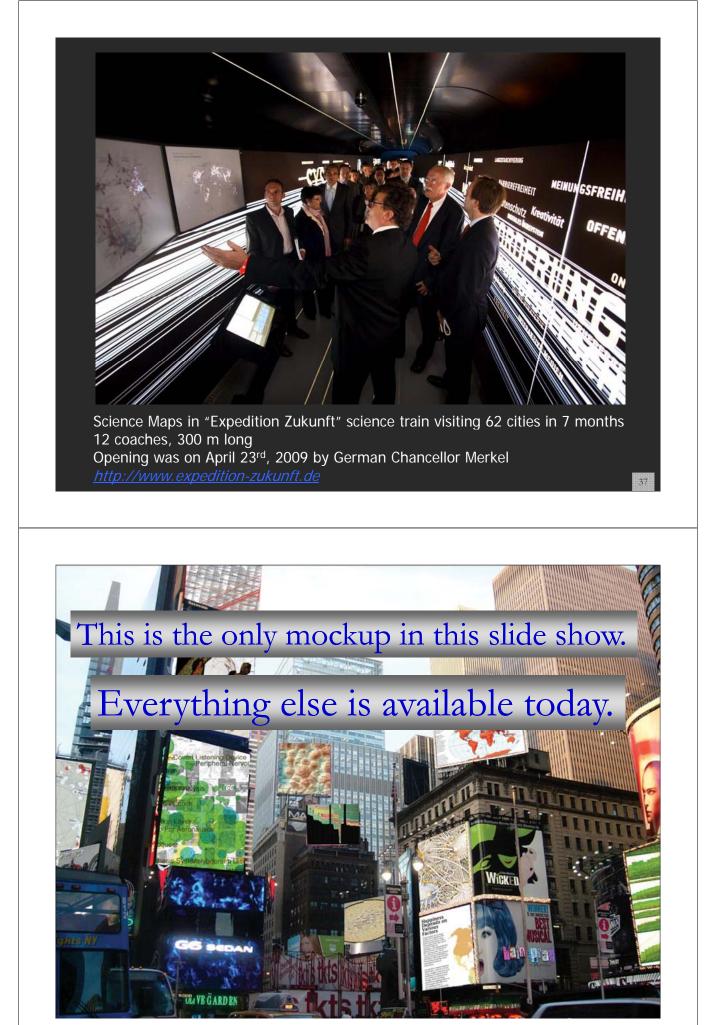
This overlay shows the distribution of nanotechnology within the paradigms of science. The majority of current work in nanotechnology takes places in physics, chemistry, and materials science, at the upper right portion of the map. However, an increasing amount of nanotechnology is being applied in the biological and medical sciences, at the lower right.

All Topics	Nanotechnology	Francis H. C. CRICK	Albert EINSTEIN	Michael E. FISHER	Susan T. FISKE
Sweep through all 776 scientific paradigms	Science on the tiny scale of molecules	Co-discovered DNA's double helix	Revitalized physics with Relativity theories	Models critical phase transitions of matter	Connects perception and stereotypes
Sustainability	Biology & Chemistry	Joshua LEDERBERG	Derek J. de Solla PRICE	Richard N. ZARE	About this display
The science behind our long-term hopes	The interface between these two vital fields	Pioneer in bacterial genetic mechanisms	Known as the "Father of Scientometrics"	Uses laser chemistry in molecular dynamics	People & organizations that helped create it





Debut of 5<sup>th</sup> Iteration of Mapping Science Exhibit at MEDIA X was on May 18, 2009 at Wallenberg Hall, Stanford University, <u>http://mediax.stanford.edu</u>, <u>http://scaleindependentthought.typepad.com/photos/scimaps</u>



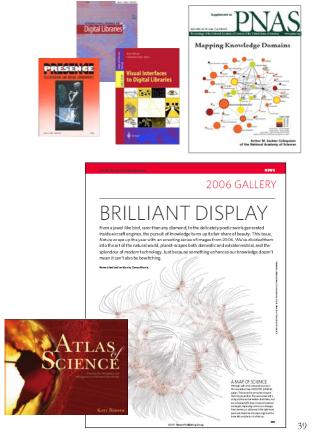
# Computational Scientometrics References

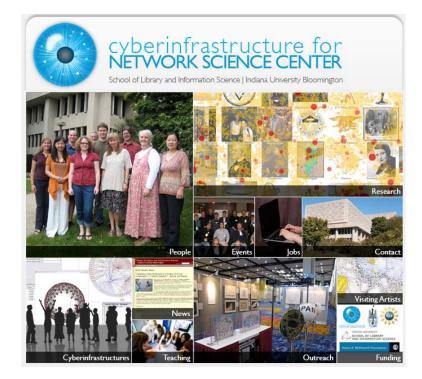
Börner, Katy, Chen, Chaomei, and Boyack, Kevin. (2003). Visualizing Knowledge Domains. In Blaise Cronin (Ed.), *ARIST*, Medford, NJ: Information Today, Inc./American Society for Information Science and Technology, Volume 37, Chapter 5, pp. 179-255. http://ivl.slis.indiana.edu/km/pub/2003-borner-arist.pdf

Shiffrin, Richard M. and Börner, Katy (Eds.) (2004). **Mapping Knowledge Domains**. Proceedings of the National Academy of Sciences of the United States of America, 101(Suppl\_1). http://www.pnas.org/content/vol101/suppl\_1/

Börner, Katy, Sanyal, Soma and Vespignani, Alessandro (2007). **Network Science.** In Blaise Cronin (Ed.), *ARIST*, Information Today, Inc./American Society for Information Science and Technology, Medford, NJ, Volume 41, Chapter 12, pp. 537-607. http://ivl.slis.indiana.edu/km/pub/2007-borner-arist.pdf

Börner, Katy (2010) Atlas of Science. MIT Press. http://scimaps.org/atlas





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