Mapping Scientific Discovery through Advanced Computing

Katy Börner

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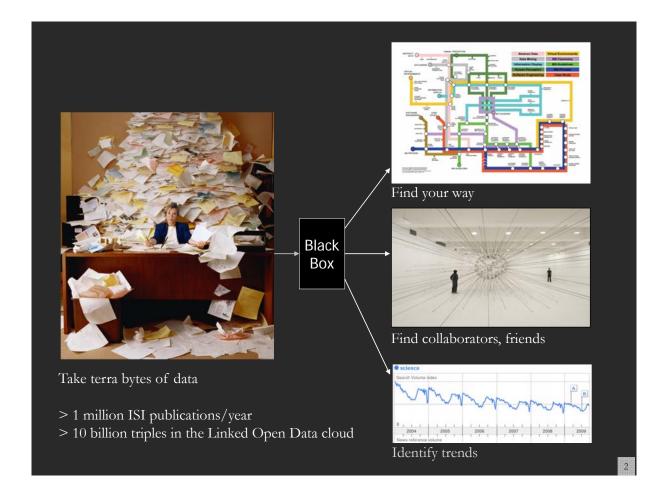




With special thanks to the members at the Cyberinfrastructure for Network Science Center, Kevin W. Boyack, the VIVO Consortium, and the Mapping Science exhibit advisory board.

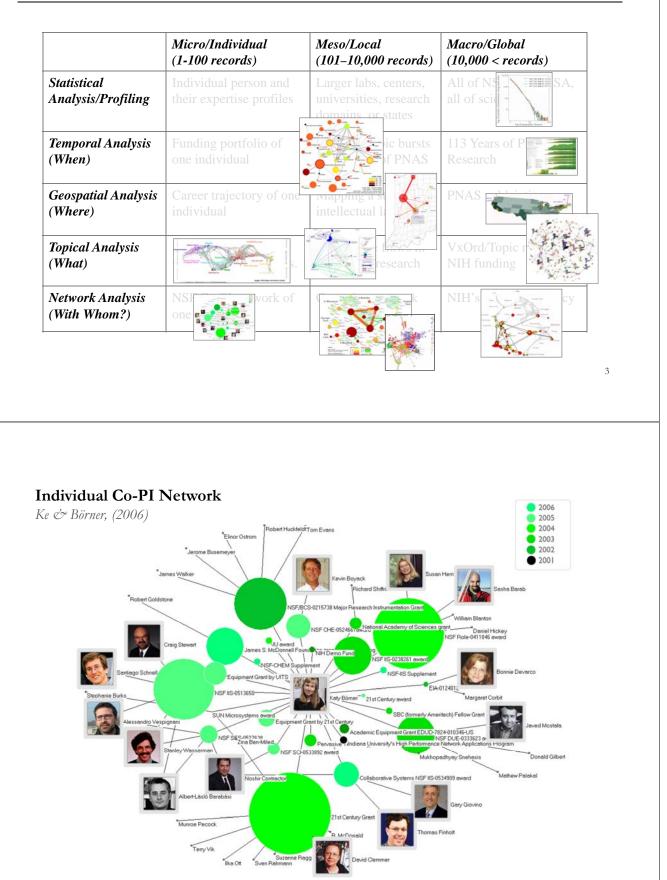
Plenary Talk at Scientific Discovery through Advanced Computing Program (SciDAC) Conference Brown Palace Hotel in Denver, Colorado

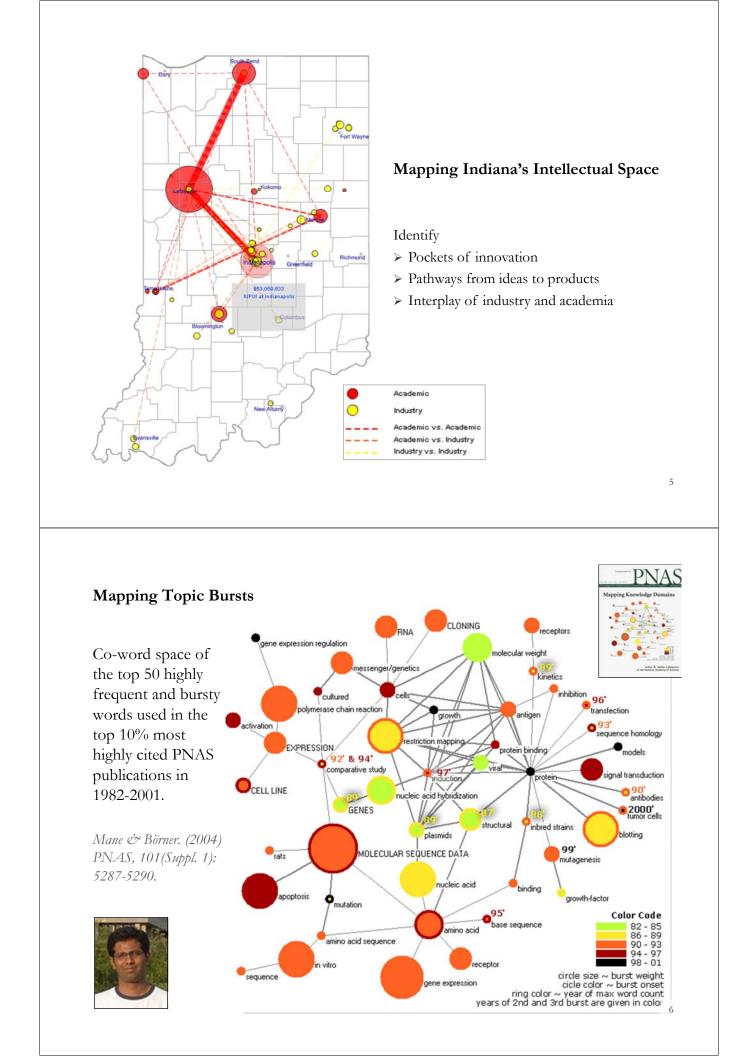
July 14, 2011

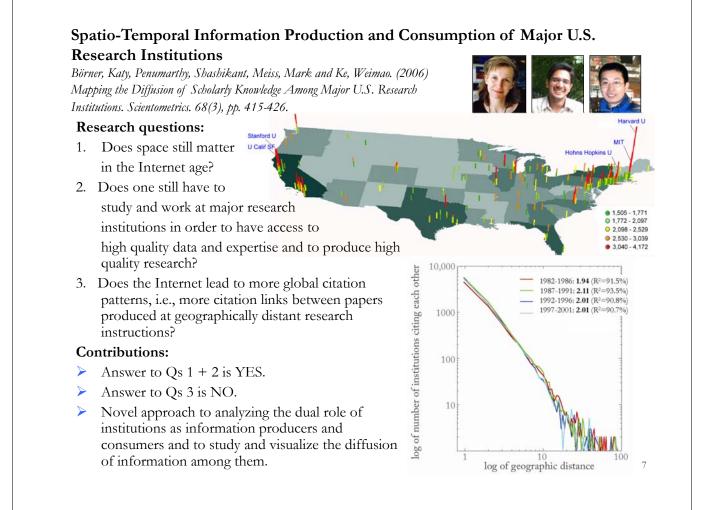




Type of Analysis vs. Level of Analysis





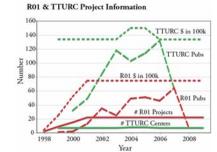


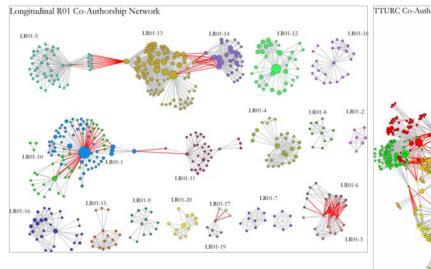
Mapping Transdisciplinary Tobacco Use Research Centers Publications

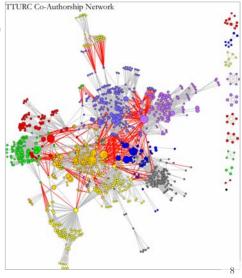
Compare R01 investigator based funding with TTURC Center awards in terms of number of publications and evolving co-author networks.

Zoss & Börner, forthcoming.

Supported by NIH/NCI Contract HHSN261200800812

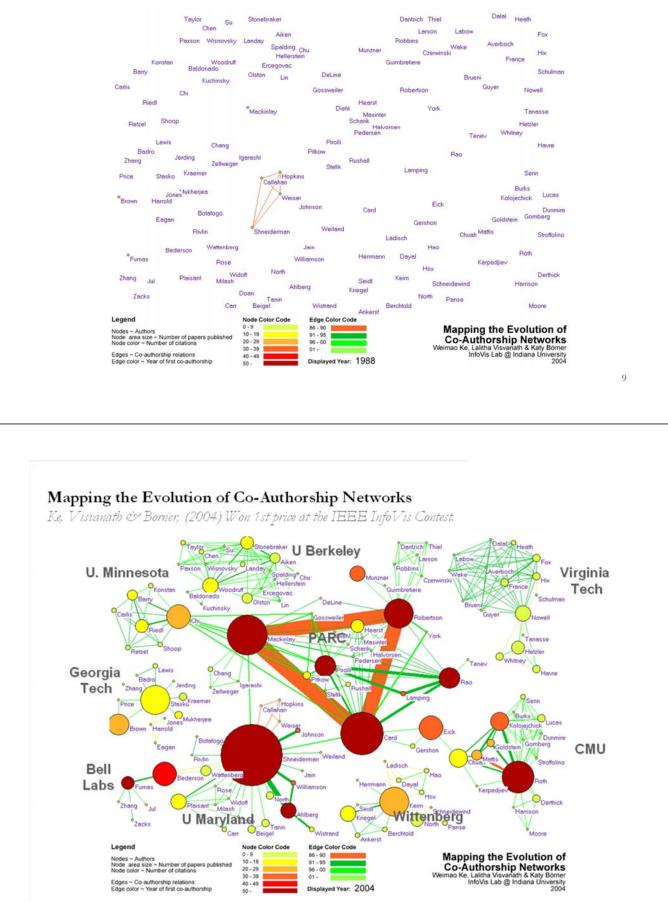






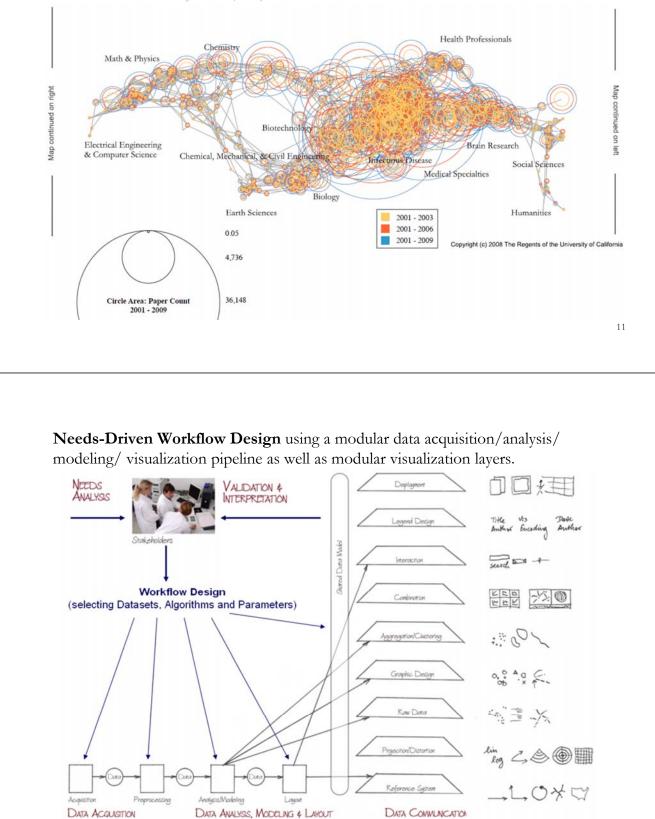
Mapping the Evolution of Co-Authorship Networks

Ke, Visvanath & Börner, (2004) Won 1st price at the IEEE InfoVis Contest.



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

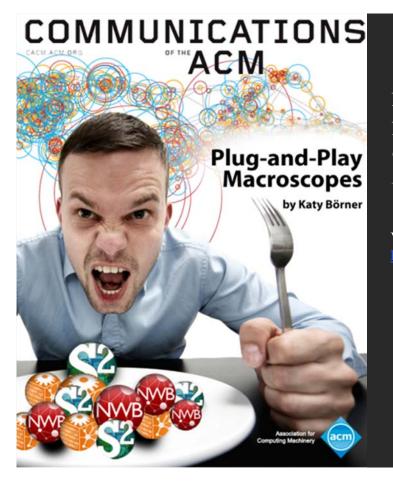
Katy Börner, Nianli Ma, Joseph R. Biberstine, Cyberinfrastructure for Network Science Center, SLIS, Indiana University, Robin M. Wagner, Rediet Berhane, Hong Jiang, Susan E. Ivey, Katrina Pearson and Carl McCabe, Reporting Branch, Division of Information Services, Office of Research Information Systems,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



\$ PREPROCESSING

Börner, Katy (2010) Atlas of Science. MIT Press. 12

VISUALIZATION LAYERS

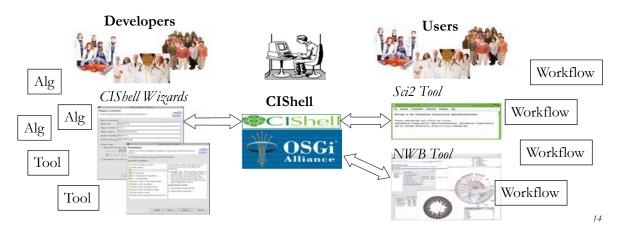


Börner, Katy. (March 2011). Plug-and-Play Macroscopes. *Communications of the ACM*, 54(3), 60-69.

Video and paper are at <u>http://www.scivee.tv/node/27704</u>

SGi & CIShell

- CIShell (<u>http://cishell.org</u>) is an open source software specification for the integration and utilization of datasets, algorithms, and tools.
- It extends the Open Services Gateway Initiative (OSGi) (<u>http://osgi.org</u>), 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 Home

@1 Added by Micah Linnemeier, last edited by Micah Linnemeier on Mar 16, 2011 (view change)

About the Cyberinfrastructure Shell

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.

CIShell is the basis of Network Workbench, TexTrend, Sci² and the upcoming EpiC tool.

CIShell supports remote execution of algorithms. A standard web service definition is in development that will allow pools of algorithms to transparently be used in a peer-to-peer, clientserver, or web front-end fashion.

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

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Learn More ...

- <u>CIShell Papers</u>
- <u>CIShell Powered Tools</u>
- <u>Algorithms</u>
- Plugins (coming soon)
- Misc. Tool Documentation
- CIShell Web Services (coming soon)
- Screenshots

Getting Started...

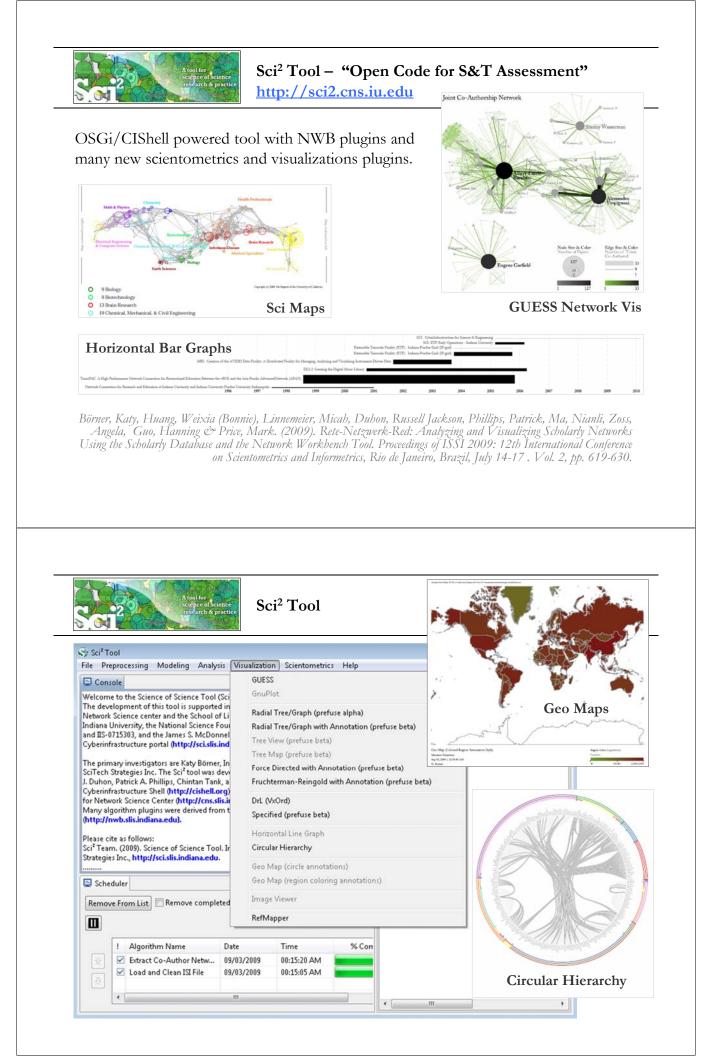
- Documentation & Developer Resources
- <u>Download</u>

Getting Involved...

<u>Contact Us</u>

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12.	Sci ² Tool A tool for science of science research & practice Email Address Password Login
Forgot your pas To recover your a Not registered y Register now	ccount password, please visit our password recovery page.
Tutorials	Katy Borner (2010) Science of Science Research and Tools (12 Tutorials). Reporting Branch, Office of Extramural Research/Office of the Director, National Institutes of Health, Bethesda, MD. • Tutorial #01: Science of Science Research • Tutorial #02: Network Science / Information Visualization • Tutorial #03: CIShell Powered Tools: Network Workbench and Science of Science Tool • Tutorial #04: Temporal Analysis – Burst Detection • Tutorial #05: Geospatial Analysis and Mapping • Tutorial #06: Topical Analysis and Visualization • Tutorial #07: Tree Analysis and Visualization • Tutorial #08: Large Network Analysis and Visualization • Tutorial #09: Large Network Analysis and Visualization • Tutorial #10: Using the Scholarly Database at IU • Tutorial #11: VIVO National Researcher Networking • Tutorial #12: Future Developments
	Geetha Senthal (2010). <u>Multidisciplinary Nature of Work With Reference to PIs and ICs Within a Portfolio</u> . PA Group at NIH. NIH Office of Extramural Research and Katy Börner (2010) <u>Network Visualizations Using SPIRES Data and the Sci2 Tool</u> . Office of Extramural Research at NIH.



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

Sci² Tool: Algorithms

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.

Extract K-Core Annotate K-Coreness ------HITS PageRank Weighted & Directed HITS

Database support for ISI and NSF data.

Weighted PageRank

Textual Burst Detection

Soon:

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

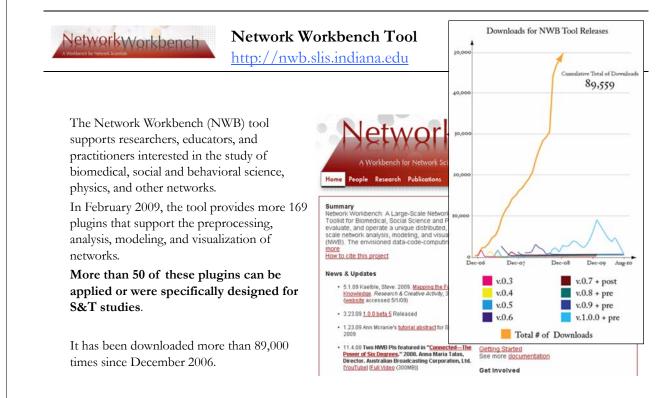
Extract Author Paper Network

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

21



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



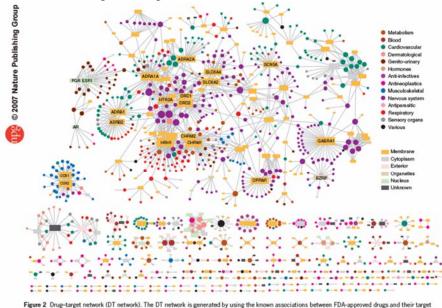


Figure 2 Drug-target network (DT network). The DT network is generated by using the known associations between FDA-approved drugs and their target proteins. Circles and rectangles correspond to drugs and target proteins, respectively. A link is placed between a drug node and a target node if the protein 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 (circle) 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.

fruits

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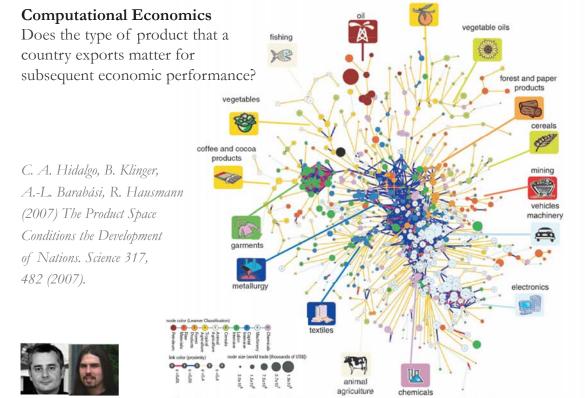


Fig. 1. The product space. (A) Hierarchically clustered proximity (a) matrix representing the 775 SITC-4 product classes exported in the 1998–2000 period. (B) Network representation of the product space. Links are color coded

with their proximity value. The sizes of the nodes are proportional to world trade, and their colors are chosen according to the classification introduced by Learner.



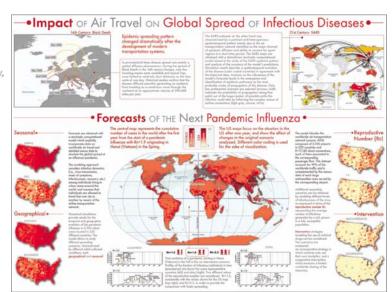
Computational Epidemics Forecasting (and preventing the effects of) the next pandemic.

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).





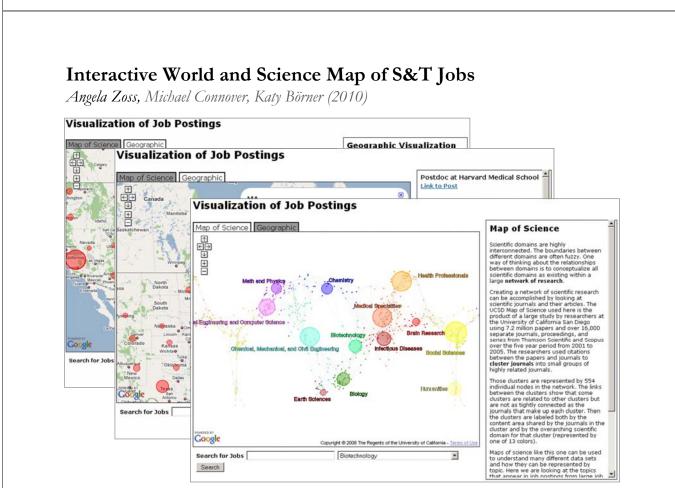


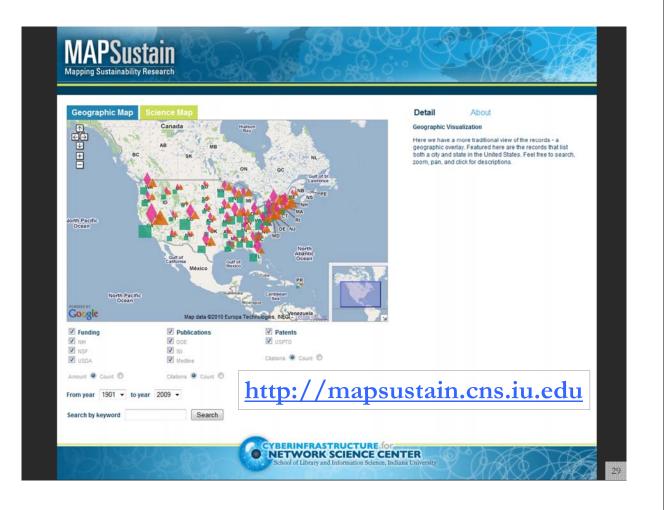
OSGi/CIShell Adoption

A number of other projects recently adopted OSGi and/or CIShell:

- Cytoscape (<u>http://cytoscape.org</u>) Led by Trey Ideker at the University of California, San Diegois 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.org.uk</u>) Developed by the myGrid team (<u>http://mygrid.org.uk</u>) led by Carol Goble at the University of Manchester, U.K. 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 (<u>https://wiki.ncsa.uiuc.edu/display/MAE/Home</u>) Managed by Jong Lee at NCSA is an open-source, extensible software platform which supports seismic risk assessment based on the Mid-America Earthquake (MAE) Center research.
- TEXTrend (<u>http://textrend.org</u>) Led by George Kampis at Eötvös Loránd University, Budapest, Hungary supports natural language processing (NLP), classification/mining, and graph algorithms for the analysis of business and governmental text corpuses with an inherently temporal component.
- DynaNets (<u>http://wmw.dynanets.org</u>) Coordinated by Peter M.A. Sloot at the University of Amsterdam, The Netherlands develops algorithms to study evolving networks.

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.







Maps Detail Data

The dataset covers 13,528 records on "biomass" and "biofuel" research and technology from seven different publication, patent, funding datasets for the years 1901 to 2010.

Funding

National Institutes of Health (NIH) awards retrieved from the Scholarly Database (http://sdb.slis.indiana.edu) at Indiana University on 11/20/2010. Search guery used was biomass OR biofuel OR "bio mass" OR "bio fuel" in the 'All Text' field.

National Science Foundation (NSF) awards retrieved from the Scholarly Database (http://sdb.slis.indiana.edu) at Indiana University on 11/20/2010. Search query used was biomass OR biofuel OR "bio mass" OR "bio fuel" in the 'All Text' field.

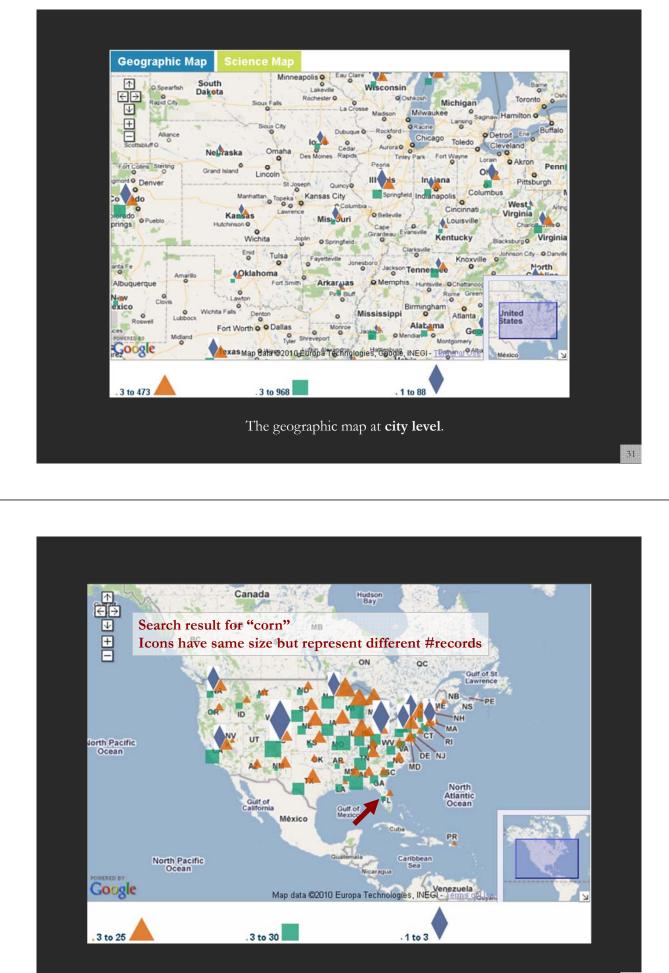
US Department of Agriculture (USDA) awards made available by a staff member of the Office of Scientific and Technical Information from the US Department of Energy (DOE).

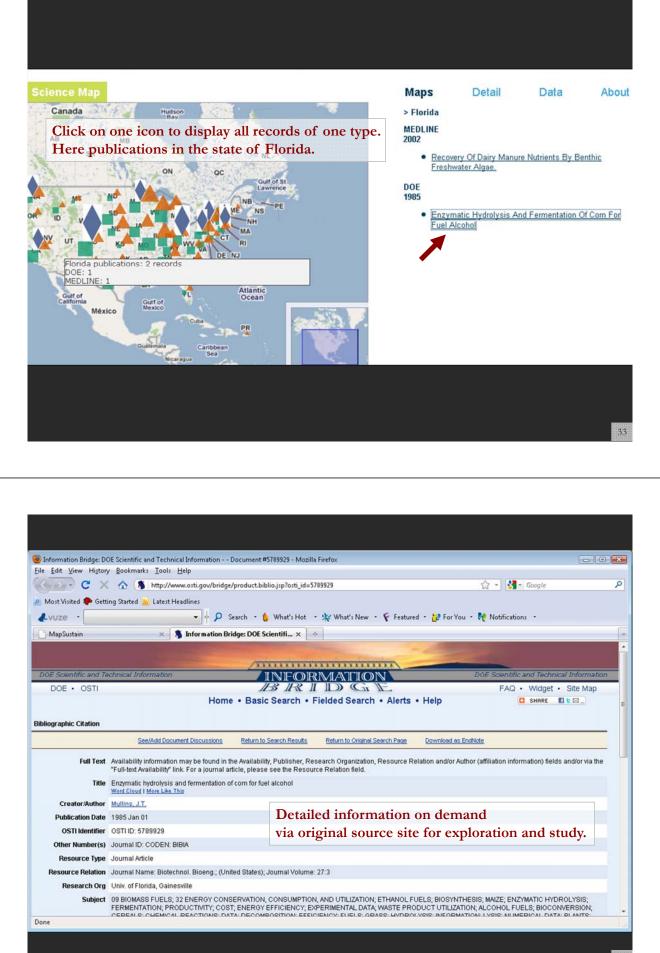
Publications

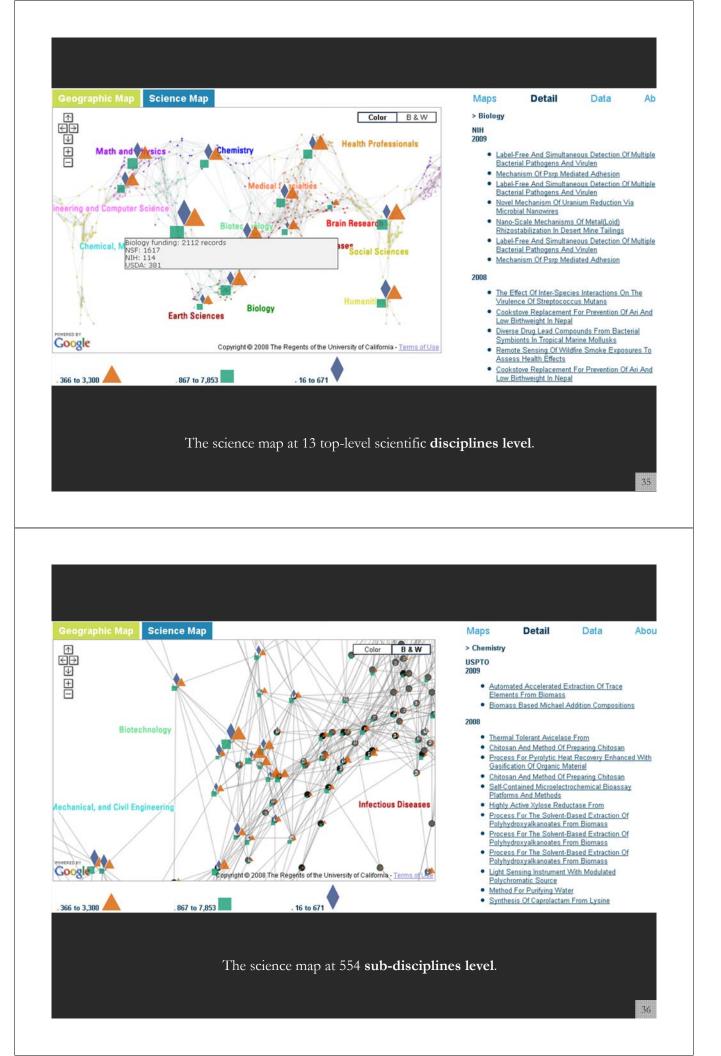
MEDLINE papers by the National Library of Medicine retrieved from the Scholarly Database (http://sdb.sils.indiana.edu) at Indiana University on 11/20/2010. Search query used was biomass OR biofuel OR "bio mass" OR "bio fuel" in the 'AII Text' field.

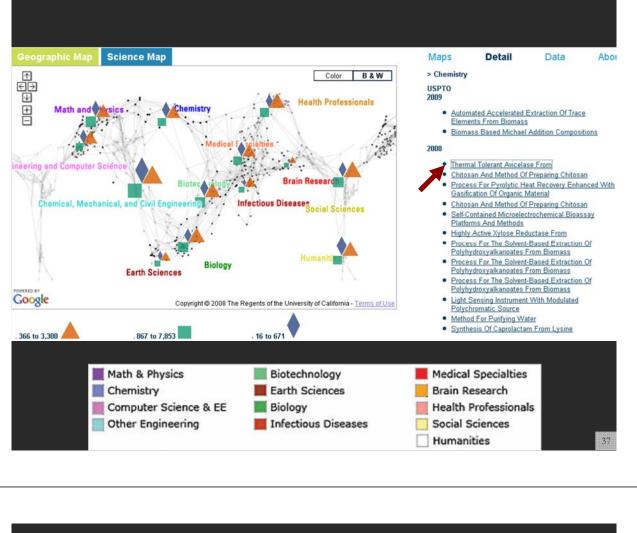
The geographic map at state level.

About

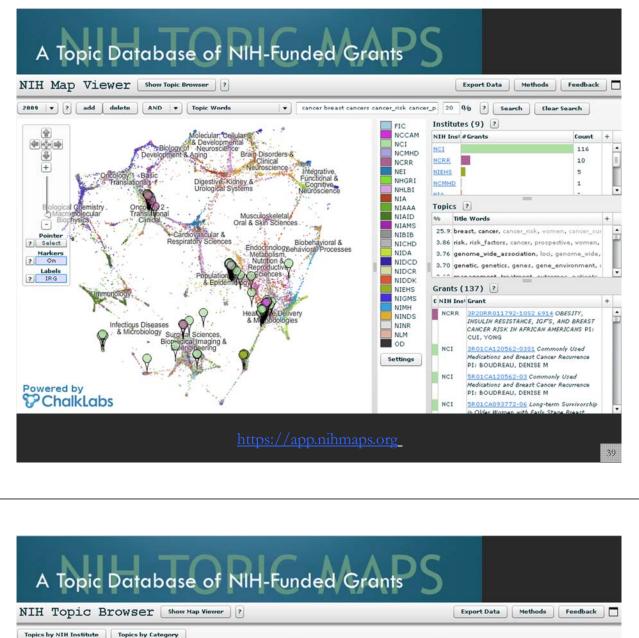








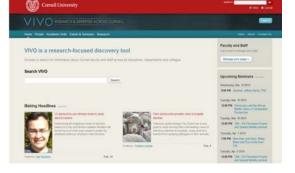
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Ding, et al.	April 2	9, 2008
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	mal tolerant (thermostable) cellulase, AviIII, that is a member of the glycoside hydrolase (GH) family. AviIII was isolated and characterized nd, like many cellulases, the disclosed polypeptide and/or its derivatives may be useful for the conversion of biomass into biofuels and chem	
nventors: Ding; S	You (Golden, CO), Adney; William S. (Golden, CO), Vinzant; Todd B. (Golden, CO), Himmel; Michael E. (Littleton, CO)	
Assignee: Midwes	Research Institute (Kansas City, MO)	
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VIVO: A Semantic Approach to Creating a National Network of Researchers (http://vivoweb.org)

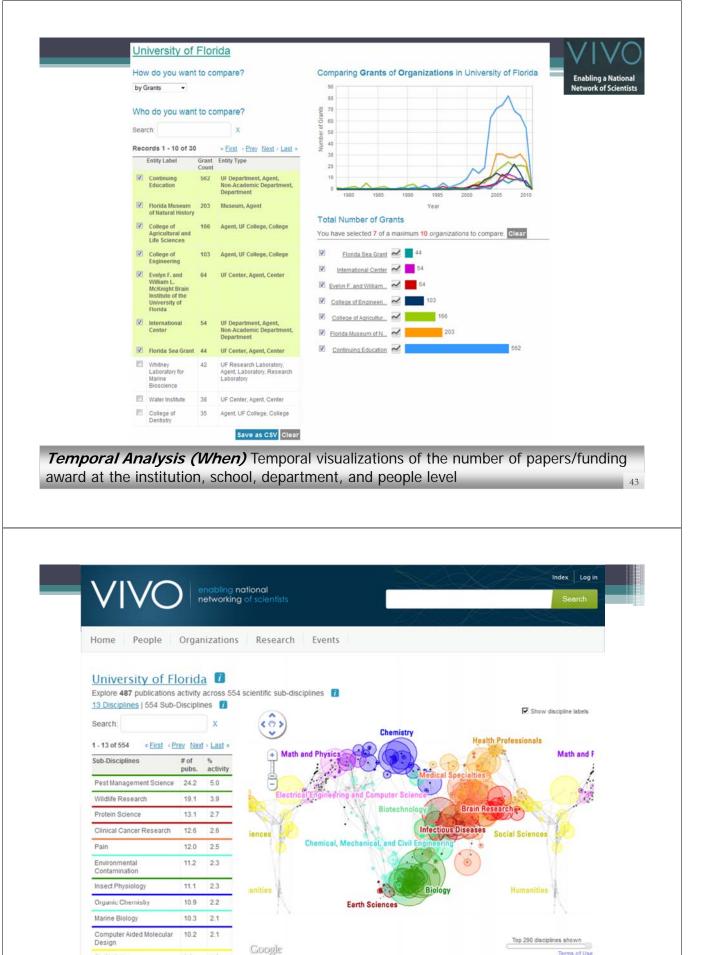
- Semantic web application and ontology editor originally developed at Cornell U.
- Integrates research and scholarship info from systems of record across institution(s).
- Facilitates research discovery and crossdisciplinary collaboration.
- Simplify reporting tasks, e.g., generate biosketch, department report.



Funded by \$12 million NIH award.

Cornell University: Dean Krafft (Cornell PI), Manolo Bevia, Jim Blake, Nick Cappadona, Brian Caruso, Jon Corson-Rikert, Elly Cramer, Medha Devare, John Fereira, Brian Lowe, Stella Mitchell, Holly Mistlebauer, Anup Sawant, Christopher Westling, Rebecca Younes. University of Florida: Mike Conlon (VIVO and UF PI), Cecilia Botero, Kerry Britt, Erin Brooks, Amy Buhler, Ellie Bushhousen, Chris Case, Valrie Davis, Nita Ferree, Chris Haines, Rae Jesano, Margeaux Johnson, Sara Kreinest, Yang Li, Paula Markes, Sara Russell Gonzalez, Alexander Rockwell, Nancy Schaefer, Michele R. Tennant, George Hack, Chris Barnes, Narayan Raum, Brenda Stevens, Alicia Turner, Stephen Williams. Indiana University: Katy Borner (IU PI), William Barnett, Shanshan Chen, Ying Ding, Russell Duhon, Jon Dunn, Micah Linnemeier, Nianli Ma, Robert McDonald, Barbara Ann O'Leary, Mark Price, Yuyin Sun, Alan Walsh, Brian Wheeler, Angela Zoss. Ponce School of Medicine: Richard Noel (Ponce PI), Ricardo Espada, Damaris Torres. The Scripps Research Institute: Gerald Joyce (Scripps PI), Greg Dunlap, Catherine Dunn, Brant Kelley, Paula King, Angela Murrell, Barbara Noble, Cary Thomas, Michaeleen Trimarchi. Washington University, St. Louis: Rakesh Nagarajan (WUSTL PI), Kristi L. Holmes, Sunita B. Koul, Leslie D. McIntosh. Weill Cornell Medical College: Curtis Cole (Weill PI), Paul Albert, Victor Brodsky, Adam Cheriff, Oscar Cruz, Dan Dickinson, Chris Huang, Itay Klaz, Peter Michelini, Grace Migliorisi, John Ruffing, Jason Specland, Tru Tran, Jesse Turner, Vinay Varughese.

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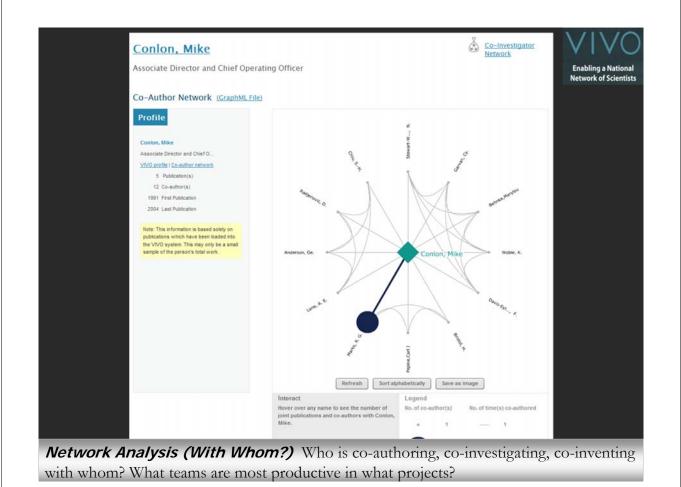


Terms of Use mapped 14.55% of 3,346 publications

Topical Analysis (What) Science map overlays will show where a person, department, or university publishes most in the world of science. (in work)

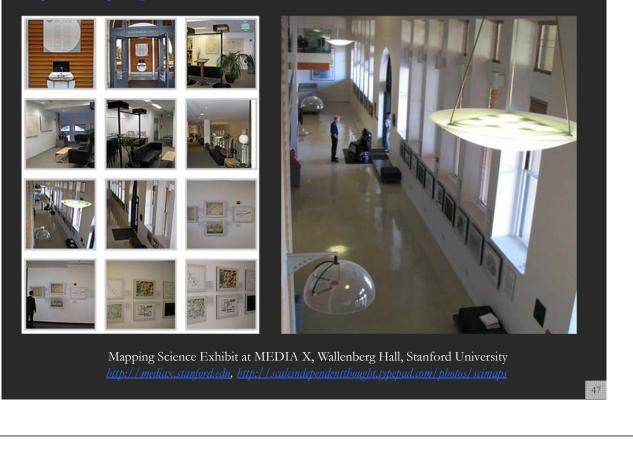
BioStatistics

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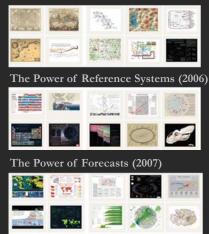
Mapping Science Exhibit – 10 Iterations in 10 years http://scimaps.org



Mapping Science Exhibit – 10 Iterations in 10 years

<u>mp.//semaps.org</u>

The Power of Maps (2005)



Science Maps for Economic Decision Makers (2008)

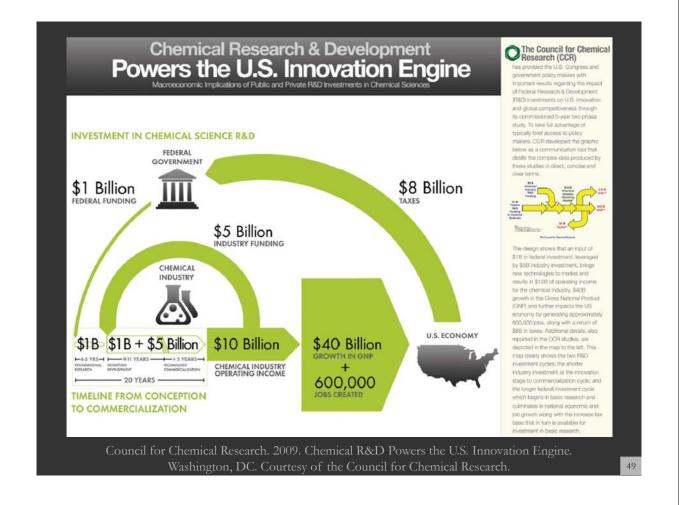
Science Maps for Scholars (2010) Science Maps as Visual Interfaces to Digital Libraries (2011) Science Maps for Kids (2012) Science Forecasts (2013) Towards Science Mapping Standards (2014)

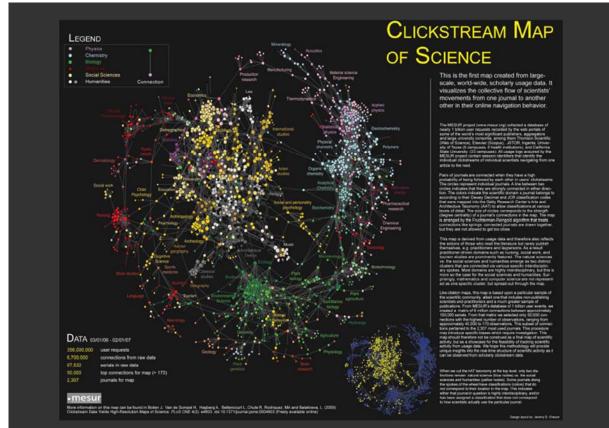
Exhibit has been shown in 72 venues on four continents. Currently at - NSF, 10th Floor, 4201 Wilson Boulevard, Arlington, VA

- Center of Advanced European Studies and Research, Bonn, German
- University of North Texas, Denton, Texas

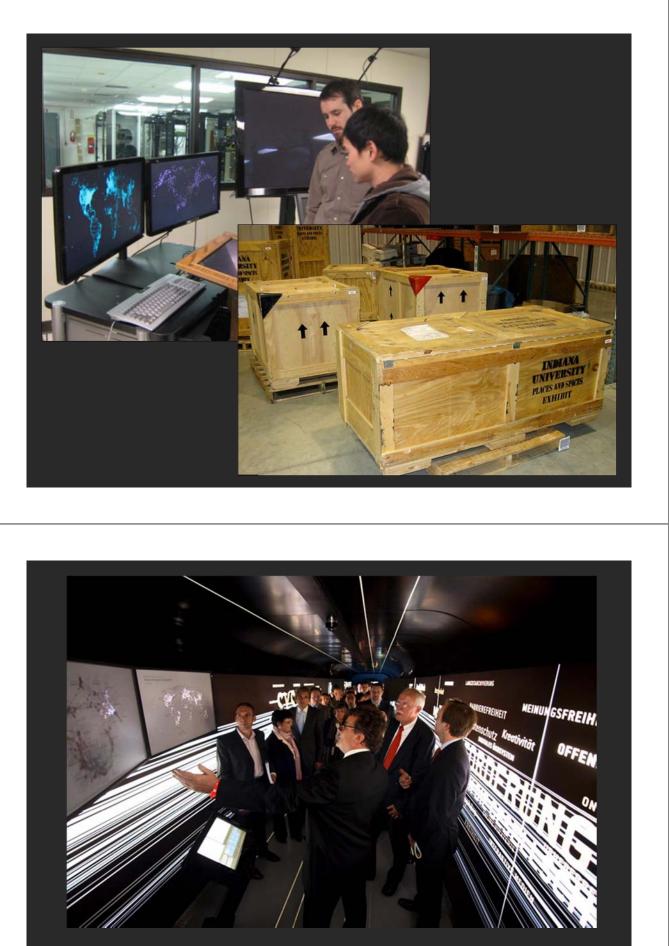








Bollen, Johan, Herbert Van de Sompel, Aric Hagberg, Luis M.A. Bettencourt, Ryan Chute, Marko A. Rodriquez, Lyudmila Balakireva. 2008. A Clickstream Map of Science. 50



Science Maps in "Expedition Zukunft" science train visiting 62 cities in 7 months, 12 coaches, 300 m long. <u>http://www.expedition-zukunft.de</u>



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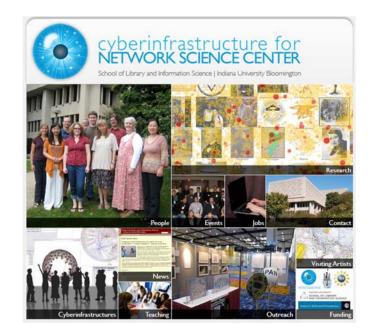
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All papers, maps, tools, talks, press are linked from http://cns.iu.edu

CNS Facebook: <u>http://www.facebook.com/cnscenter</u> Mapping Science Exhibit Facebook: <u>http://www.facebook.com/mappingscience</u>