Plug-and-Play Macroscopes

Dr. Katy Börner

Cyberinfrastructure for Network Science Center, Director Information Visualization Laboratory, Director School of Library and Information Science Indiana University, Bloomington, IN katy@indiana.edu

With special thanks to the members at the Cyberinfrastructure for Network Science Center and the Mapping Science exhibit map makers and advisory board members, and the NWB and Sci2 team.

Beyond Open Access: The Wiki-era, Translational Medicine, and Scientometrics 3rd European Conference on Scientific Publishing in Biomedicine and Medicine (ECSP3) Leiden University Medical Center, The Netherlands

- Center of Advanced European Studies and Research, Bonn, Germany

ORDER









Debut of 5th 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>





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 or 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.



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 Macroscopes

- *Core Architecture & Plugins/Division of Labor:* Computer scientists need to design the standardized, modular, easy to maintain and extend "core architecture". Dataset and algorithm plugins, i.e., the "filling", are 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. Users need guidance for constructing effective workflows from 100+ continuously changing plugins.
- *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 (industry) 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.



Example: Science of Science Studies

About 5-20 algorithms are involved in one single study/workflow.



Börner, Katy, Chen, Chaomei, and Boyack, Kevin. (2003) Visualizing Knowledge Domains. ARIST, pp. 179-255.

Domain has about 300 core researchers, 10 key data sources, 20 common tools.

Approaches/algorithms from network science, social science, political science, economics, physics, information science, webometrics, etc. are highly relevant and new ones become available every day.

2002 Base Map of Science

Kevin W. Boyack, Katy Börner, & Richard Klavans (2007). Mapping the Structure and Evolution of Chemistry Research. 11th International Conference on Scientometrics and Informetrics. pp. 112-123.

- Uses combined SCI/SSCI from 2002
 - 1.07M papers, 24.5M references, 7,300 journals
 - Bibliographic coupling of papers, aggregated to journals
- Initial ordination and clustering of journals gave 671 clusters
- Coupling counts were reaggregated at the journal cluster level to calculate the
 - (x,y) positions for each journal cluster
 - by association, (x,y) positions for each journal



Science map applications: Identifying core competency

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



Funding patterns of the US Department of Energy (DOE)

Infectious Diseases

Virology

Science map applications: Identifying core competency

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



Funding Patterns of the National Institutes of Health (NIH)



Macroscope Design





Network Workbench Tool + Community Wiki http://nwb.slis.indiana.edu Science of Science (Sci²) Tool and Portal

Custom Tools for Different Scientific Communities Information Visualization Cyberinfrastructure http://iv.slis.indiana.edu

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

180+ Algorithm Plugins and Branded GUIs

+**Core Architecture**

Open Services Gateway Initiative (OSGi) Framework. http://orgi.org Cyberinfrastructure Shell (CIShell) http://cishell.org







Cyberinfrastructure Shell (CIShell) **C**IShel http://cishell.org > CIShell 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://www.osgi.org</u>), a standardized, component oriented, computing environment for networked services widely used in industry since 10 years. Specifically, CIShell provides "sockets" into which existing and new datasets, algorithms, and tools can be plugged using a wizard-driven process. Developers Users IV Tool CIShell Wizards **CIShell** IShel 30 DSGi NWB Interface Allianc 17 NetworkWorkbench Network Workbench Tool http://nwb.slis.indiana. NWB Downloads Cummulative 70.000 Oct 2006-Eeb 2010 60,000 The Network Workbench (NWB) tool 50.000 supports researchers, educators, and 40,000 practitioners interested in the study of

biomedical, social and behavioral science, 30,000 physics, and other networks. Summary In February 2009, the tool provides more 169 20,000 Network Workbench: Toolkit for Biomedica evaluate, and operati scale network analysi (NWB). The envision plugins that support the preprocessing, analysis, modeling, and visualization of 10,000 more How to cite this proje networks. News & Updates 2007-8 2008-1 2008-6 2008-6 2008-11 More than 50 of these plugins can be 2009-9 2009-4 2010-2 2007 2006 5.1.09 Kaelble : applied or were specifically designed for <u>Knowledge</u>, *Rese* (<u>website</u> accesse S&T studies. Time 3.23.09 1.0.0 beta 5 Released Windows (XP & Vista) 💌 DOWNLOA 1.23.09 Ann Mcranie's <u>tutorial abstract</u> for Sunbelt 2009 It has been downloaded more than 65,000 11.4.08 Two NWB PIs featured in "<u>Connected—The</u> <u>Power of Six Degrees</u>," 2008. Anna Maria Talas, Director. Australian Broadcasting Corporation, Ltd. [YouTube] [Euli Video (300MB)] Getting Started See more documentation times since December 2006. Get involved

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 (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.





Fig. 1. The product space. (A) Hierarchically clustered proximity (ϕ) 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 Leamer.



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).





NetworkWorkbench **NWB** Tool Interface Components 🐵 Network Workbench Tool File Preprocessing Modeling Analysis Visualization Scientometrics Help - -📮 Console 🛛 🗕 100 Data Manager - -Console displays data operations (save, load, view, etc.) and Welcome to the Netwo preprocessing, modeling, analysis, and ~ algorithm input parameters, visualization of small, r selection, & acknowledgements as The Network Workben well as error reporting. is supported in part by the NSF Data Manager keeps track of all datasets that are available IIS-0513650 award. The primary investigators are от кату 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 Thalres, Soma Sanyal, Ann McCranie, Alessandro Vespignani, and Katy Börner. It uses the Cyberinfrastructure Shell (http://cinsell.org) developed at the Cyberinfrastructure for Network Science Center (http://cins.slis.indiana.edu) at Indiana University. Please cite as follows: NWB Team. (2006). Network Workbench Tool. Indiana University and Northeastern University, http://nwb.slis.indiana.edu ¥ Table Scheduler lists what algorithms you've - 8 📃 Scheduler 🔸 Matrix used and displays algorithm W progress. Plot Remove From List e all completed =× Text Ш G GUESS Algorithm Name Date % Complete Time Tree Û 🖏 Network-Ŷ Console shows references to seminal works. Workflows are recorded into a log file, and soon can be re-run for easy replication. All algorithms are documented online; workflows are given in tutorials. 23

Networkworkbench NWB Tool: Supported Data Formats

Personal Bibliographies

- Bibtex (.bib)
- 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
- NIH funding awards by the National Institutes of Health (NIH)
- NSF funding awards by the National Science Foundation (NSF)
- U.S. patents by the United States Patent and Trademark Office (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)

NetworkWorkbench

NWB Tool: Algorithms (July 1st, 2008)

See https://nwb.slis.indiana.edu/community and handout for details.

Visualization Edit

Tools

Preprocessing Edit

Remove Nodes Extract Top Nodes Extract Nodes Above or Below Val Delete High Degree Nodes Delete Random Nodes Delete Isolates Remove Edges Extract Top Edges Extract Edges Above or Below Val Remove Self Loops Trim By Degree? Pathfinder Network Scaling Sampling Snowball Sampling (n nodes) Node Sampling Edge Sampling Transformations Symmetrize Dichotomize

Multipartite Joining

Modeling Edit

General Random Graph Watts-Strogatz Small World Barabási-Albert Scale-Free Structured CAN Chord Unstructured Hypergrid PRU Other TARL Discrete Network Dynamics

Analysis Edit **General Purpose** Network Analysis Toolkit² **Unweighted & Undirected** Based on degree/ Node Degree Node Distribution Based on clustering k-Nearest Neighbor Watts Strogatz Clustering Coefficie Watts Strogatz Clustering Coefficie Based on path Diameter Average Shortest Path Shortest Path Distribution Node Betweenness Centrality Based on components Connected Components Weak Component Clustering K-Core Extract K-Core? Annotate K-Coreness? **Unweighted & Directed** Based on degree Node Indegree Node Outdearee Indegree Distribution Outdegree Distribution Based on local graph structure k-Nearest Neighbor Single Node In-Out Degree Correla

Unnamed Category? Page Rank Based on local graph structure Dyad Reciprocity? Arc Reciprocity?

GUESS <u>GnuPlot</u>? Predefined Positions Layout DrL (VxOrd) Pre-defined Positions (prefuse beta)? Move Circular Tree Layouts Radial Tree (prefuse alpha) Radial Tree with Annotations (prefuse beta)? Tree Map Tree View Balloon Graph (prefuse alpha)² Network Layouts Force Directed with Annotation (prefuse beta) Kamada-Kawai (JUNG) Fruchterman-Reingold (JUNG) Fruchterman-Reingold with Annotation (prefuse beta) Spring (JUNG) Small World (prefuse alpha) **Other Layouts**

Parallel Coordinates (demo)? LaNet (k-Core Decomposition)

Scientometrics

Extract Network From Table Extract Co-Authorship Network Extract Co-Occurrence Network From Table? Extract Directed Network From Table Extract Network From Another Network Extract Bibliographic Coupling Similarity Network Extract Co-Citation Similarity Network² Cleaning Remove ISI Duplicate Records

NetworkWorkbench NWB Tool: Output Formats

- NWB tool can be used for data conversion. Supported output formats comprise:
- ► CSV (.csv)
- ► NWB (.nwb)
- Pajek (.net)
- 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.





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

- Explicitly designed for SoS research and practice, well documented, easy to use.
- Empowers many to run common studies while making it easy for exports to perform novel research.
- Advanced algorithms, effective visualizations, and many (standard) workflows.
- Supports micro-level documentation and replication of studies.
- Is open source—anybody can review and extend the code, or use it for commercial purposes.

OPINION

nature

- Existing metrics have known flaws
 A reliable, open, joined-up data infrastructure is needed
- Data should be collected on the full
- range of scientists' work
- Social scientists and economists
- should be involved

Let's make science metrics more scientific

To capture the essence of good science, stakeholders must combine forces to create an open, sound and consistent system for measuring all the activities that make up academic productivity, says **Julia Lane**.

 $2\overline{7}$

Vol 464|25 March 2010



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.





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

Sci² Tool: Algorithms

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

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

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

Database support for ISI and

Textual Burst Detection

NEW:

NSF data.

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. Automatic legends.

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

31

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.



Year

2000



Interactive Science Map of NIH Funding

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



http://cns-nd3.slis.indiana.edu/mapjobs/geo

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





Discussion and Outlook

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* (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* (<u>https://wiki.ncsa.uiuc.edu/display/MAE/Home</u>) 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** (<u>http://www.textrend.org</u>) 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.



Discussion & Outlook cont.

Star Scientist -> Research Teams might have 100 or more members & exist few months only. **Users -> Contributors** students, faculty, practitioners.

Disciplinary -> Cross-disciplinary with different cultures, languages, approaches. **One Specimen -> Data Streams** updated nightly or even more frequently

High Quality Open Data

Scholarly Database: 23 million scholarly records



<u>http://sdb.slis.indiana.edu</u>
 VIVO National Researcher Networking

http://vivoweb.org

Static Instrument -> Evolving Cyberinfrastructure (CI) daily learning and documentation.

Macroscopes can make a major difference if they support:

Division of Labor – proper incentive structures are key.
Ease of Use – learn from YouTube, Flickr, Wikipedia
Modularity – plug-and-play helps reduce costs; increases flexibility, augmentation, customization
Standardization – speeds up 'translation' into products/practice.
Open Data and Open Code – use the minds of millions!



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