Visualization Insights from Big Data: Envisioning Science, Engineering, and Innovation

Friday, 13 February 2015: 8:00 AM-9:30 AM
Room LL20D (San Jose Convention Center)

Advanced data mining and visualization techniques can be used to extract patterns and trends from large and complex datasets. Resulting visualizations help manage, navigate, and understand vast amounts of information; support new discoveries and questions; and are a great tool to communicate science to a general audience. This interdisciplinary session brings together experts from chemistry, engineering, science policy, and art to showcase visual solutions that are instrumental in achieving high return on investment; science mapmakers who use visual analytics to identify emerging areas of research and innovation, calculate the impact of science policy interventions, and predict science and technology trends; and visual techniques that render the abstract into the concrete using computer graphics and cinematic approaches. This session will be extremely visual to highlight novel information mining and imaging techniques that enhance understanding and improve daily decision-making.

Organizer: *Katy Borner, Indiana University*

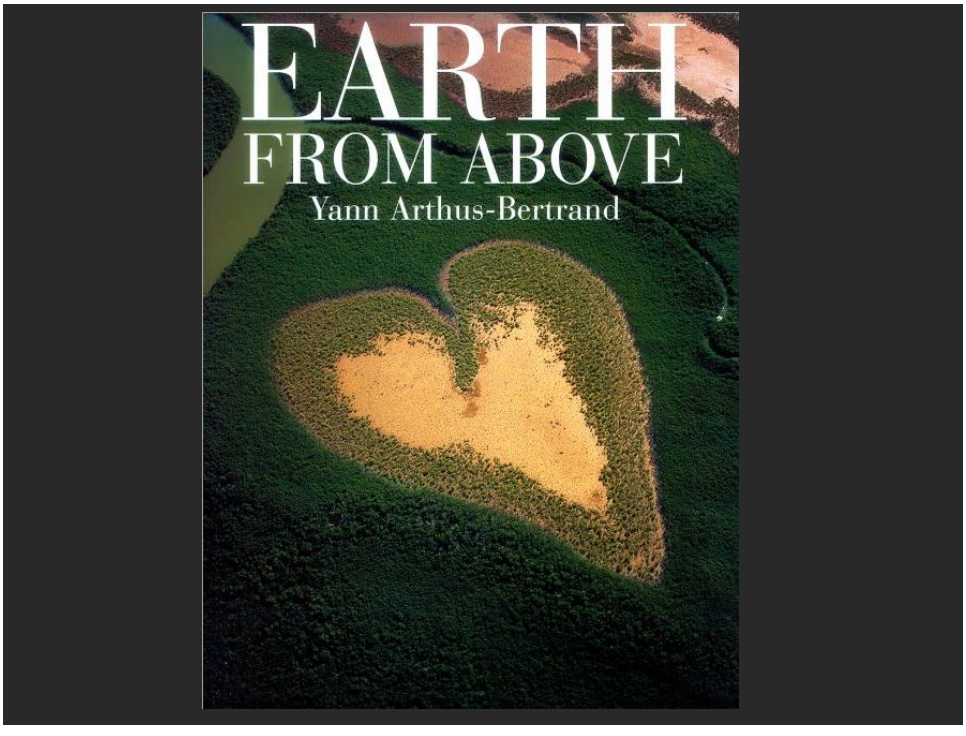
Co-Organizer: *Joseph E. Sabol, Chemical Consultant*

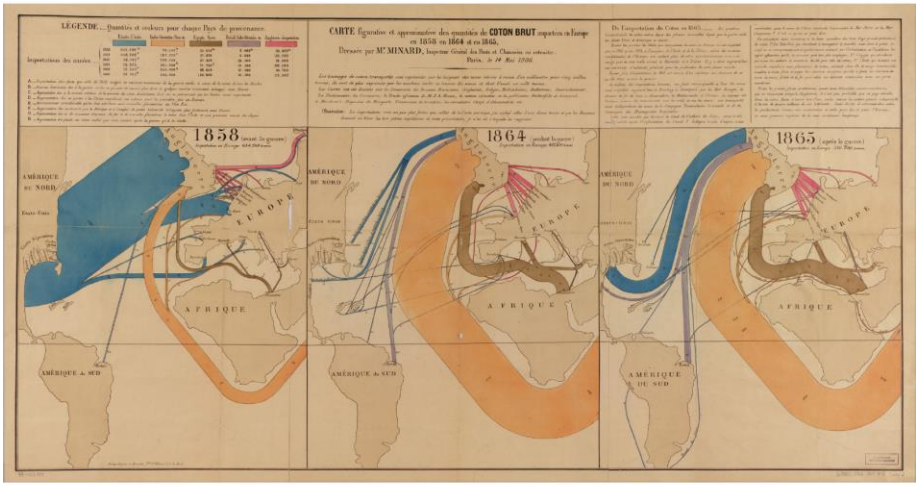
Speakers:

***Alan Aspuru-Guzik**, Harvard University*
Billions and Billions of Molecules: Exploring Chemical Space for New Energy Materials

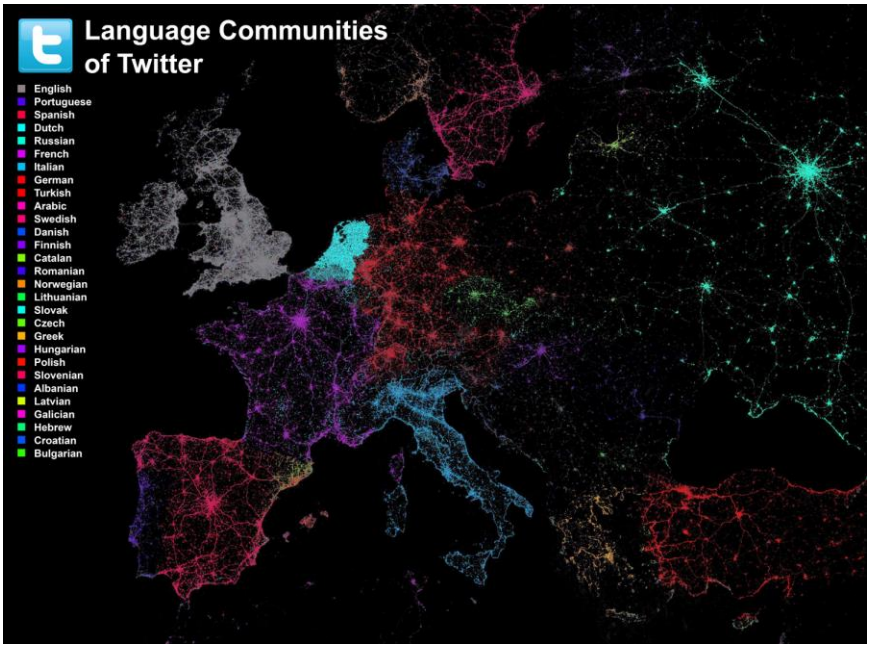
***Kei Koizumi**, U.S. Office of Science and Technology Policy*
Utilizing Visual Insights in Science and Technology Policymaking

***Donna Cox**, National Center for Supercomputing Applications*
The Art of Visualizing Big Data

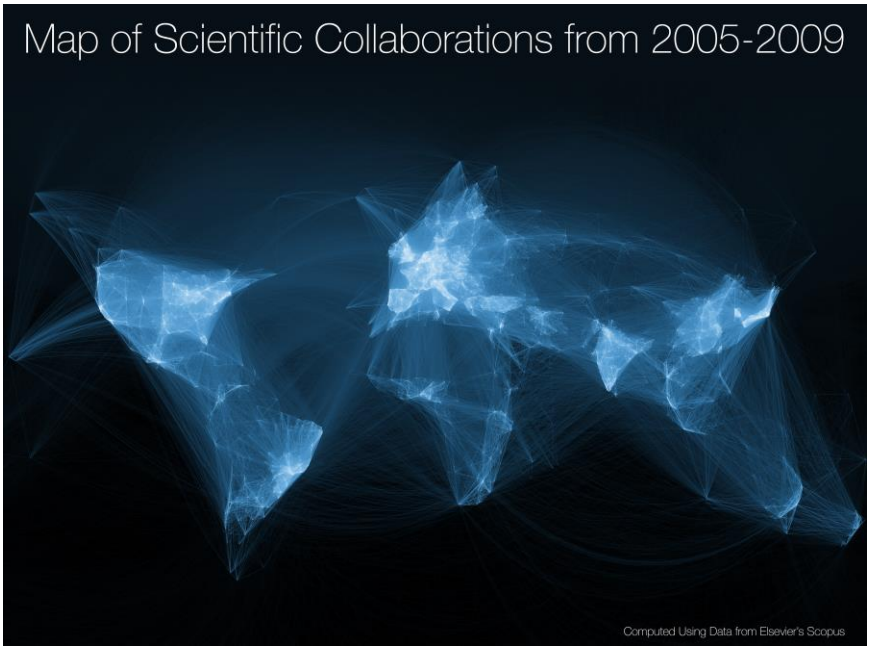




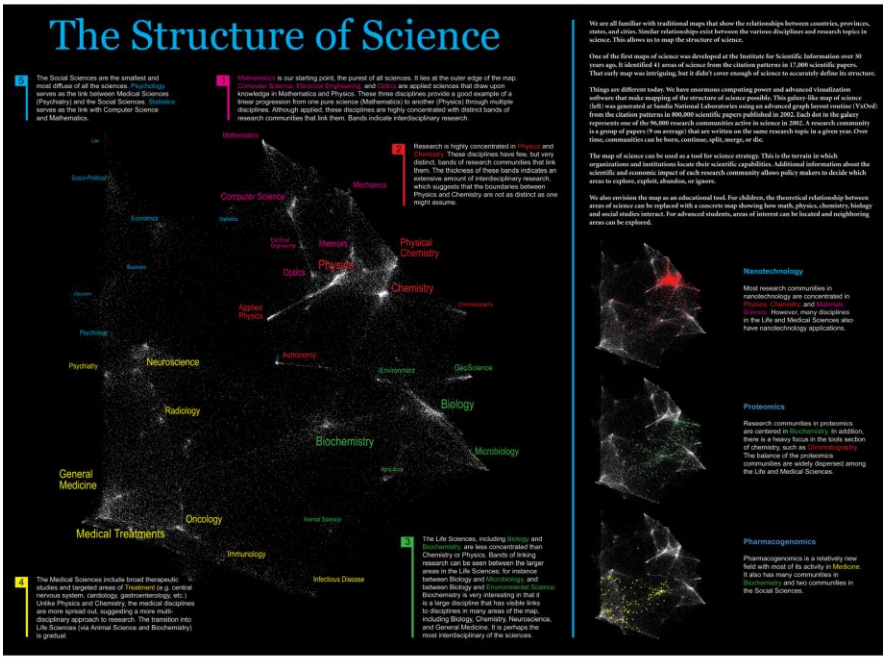
Europe Raw Cotton Imports in 1858, 1864 and 1865 - Charles Joseph Minard - 1866



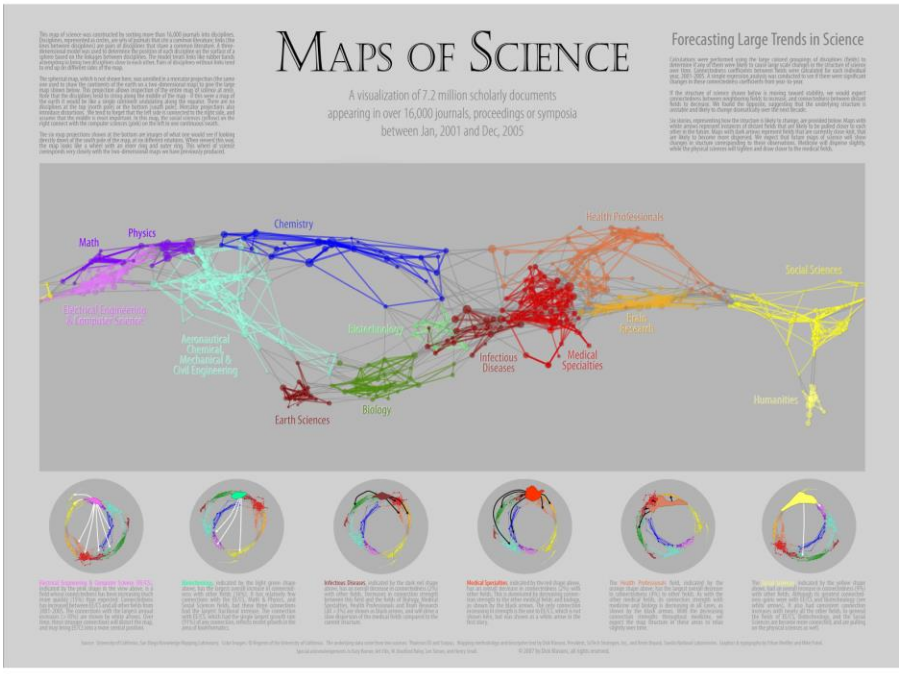
Language Communities of Twitter - Eric Fischer - 2012



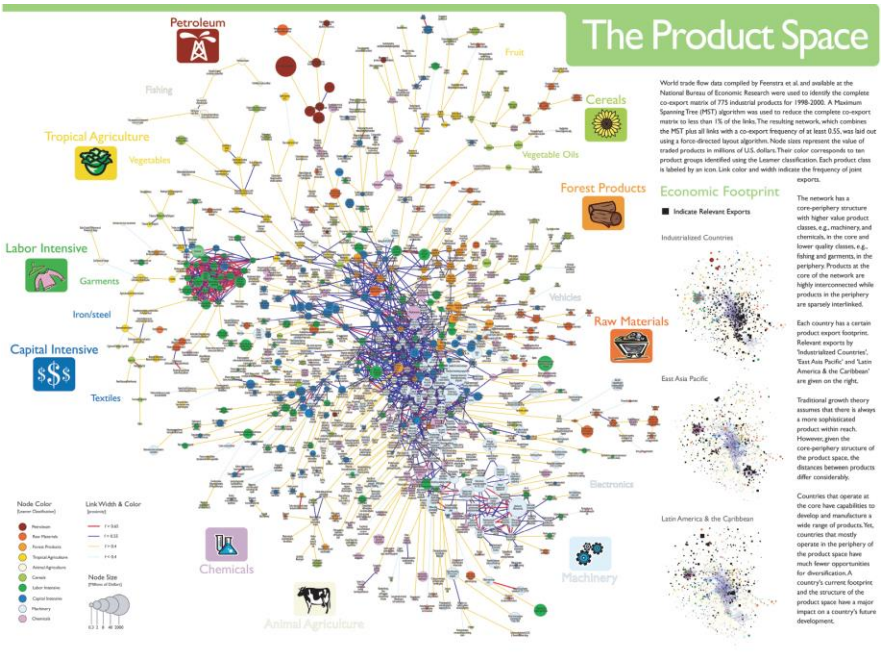
Stream of Scientific Collaborations between World Cities - Olivier H. Beauchesne - 2012



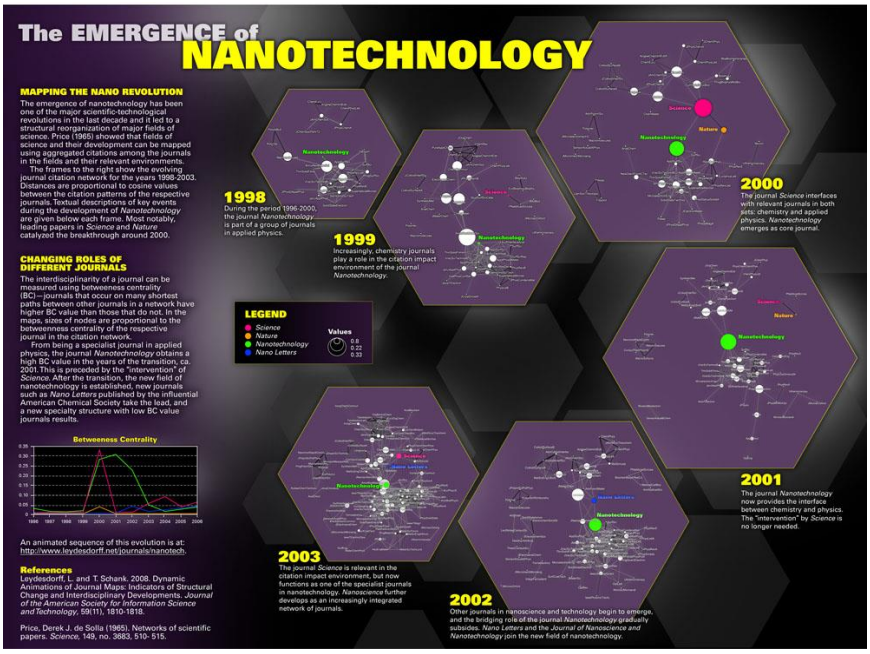
The Structure of Science - Kevin Boyack, Richard Klavans - 2005



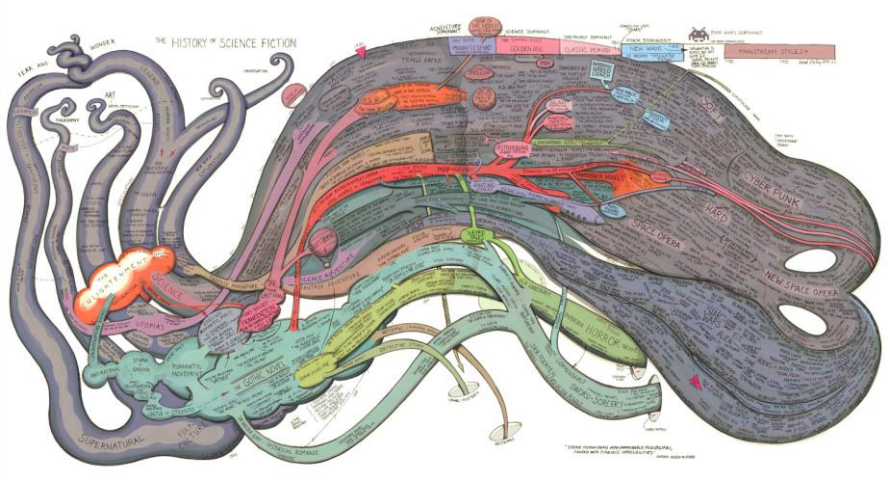
Maps of Science: Forecasting Large Trends in Science - Richard Klavans, Kevin Boyack - 2007



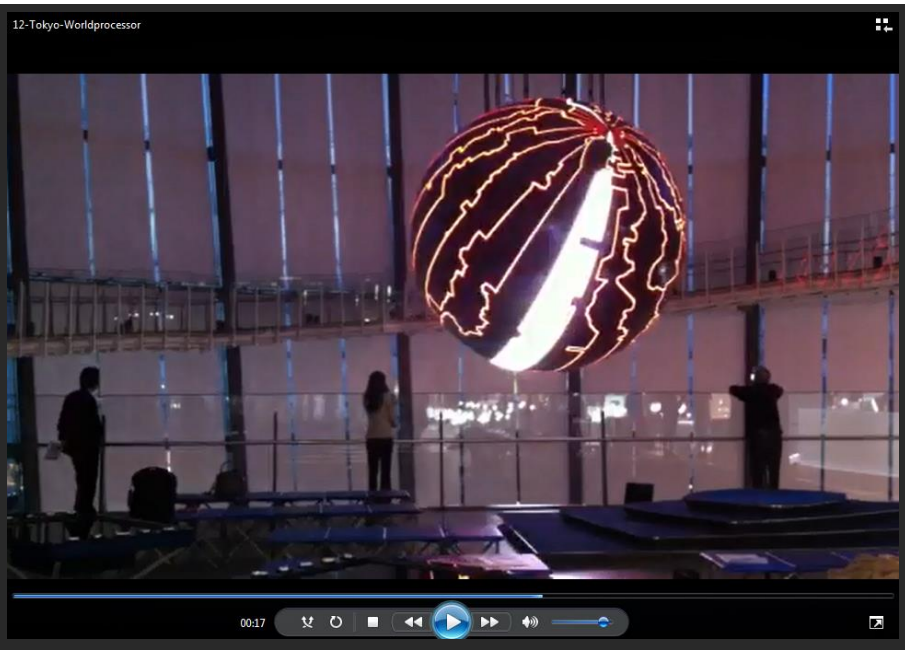
The Product Space - Cesar A. Hidalgo, Bailey Klinger, Albert-Laszlo Barabasi, Ricardo Hausmann - 2007



The Emergence of Nanoscience & Technology - Loet Leydesdorff - 2010

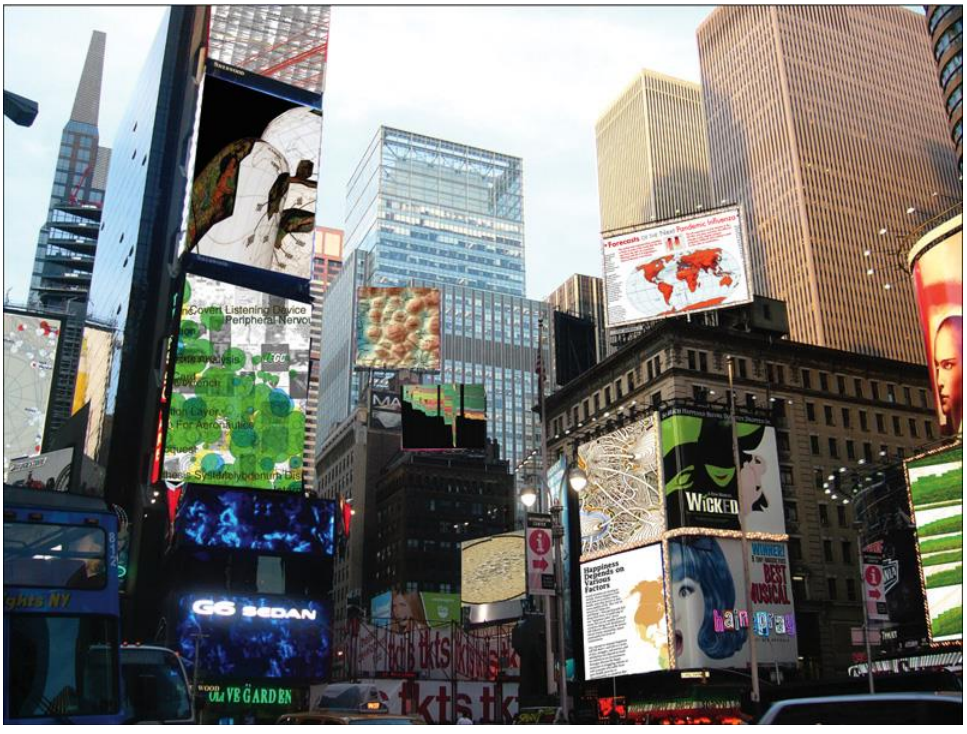


History of Science Fiction - Ward Shelley - 2011



Ingo Gunther's Worldprocessor globe design on display at the Giant Geo Cosmos OLED Display at the Museum of Emerging Science and Innovation in Tokyo, Japan

Science Maps in "Expedition Zukunft" science train visiting 62 cities in 7 months, 12 coaches, 300 m long. Opening was on April 23rd, 2009 by German Chancellor Merkel, *http://www.expedition-zukunft.de*



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Börner, Katy, Chen, Chaomei, and Boyack, Kevin. (2003). **Visualizing Knowledge Domains.** In Blaise Cronin (Ed.), *ARIST*, Medford, NJ: Information Today, 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 (2010) **Atlas of Science: Visualizing What We Know**. The MIT Press. http://scimaps.org/atlas

Scharnhorst, Andrea, Börner, Katy, van den Besselaar, Peter (2012) **Models of Science Dynamics**. Springer Verlag.

Katy Börner, Michael Conlon, Jon Corson-Rikert, Cornell, Ying Ding (2012) **VIVO: A Semantic Approach to Scholarly Networking and Discovery**. Morgan & Claypool.

Katy Börner and David E Polley (2014) **Visual Insights: A Practical Guide to Making Sense of Data**. The MIT Press.

Börner, Katy (2015) **Atlas of Knowledge: Anyone Can Map**. The MIT Press. http://scimaps.org/atlas2

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The Art of Visualizing Big Data

Billions and Billions of Molecules

Exploring Chemical Space for Energy Materials

Alán Aspuru-Guzik
Professor of
Chemistry and Chemical Biology
Harvard University

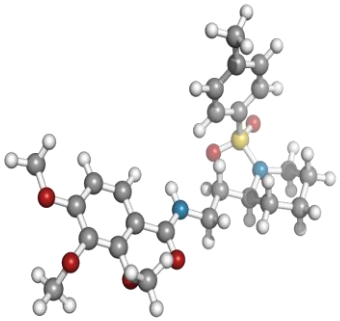
http://aspuru.chem.harvard.edu
Twitter: **A_Aspuru_Guzik**
aspuru@chemistry.harvard.edu

Some of the challenges of the 21st century

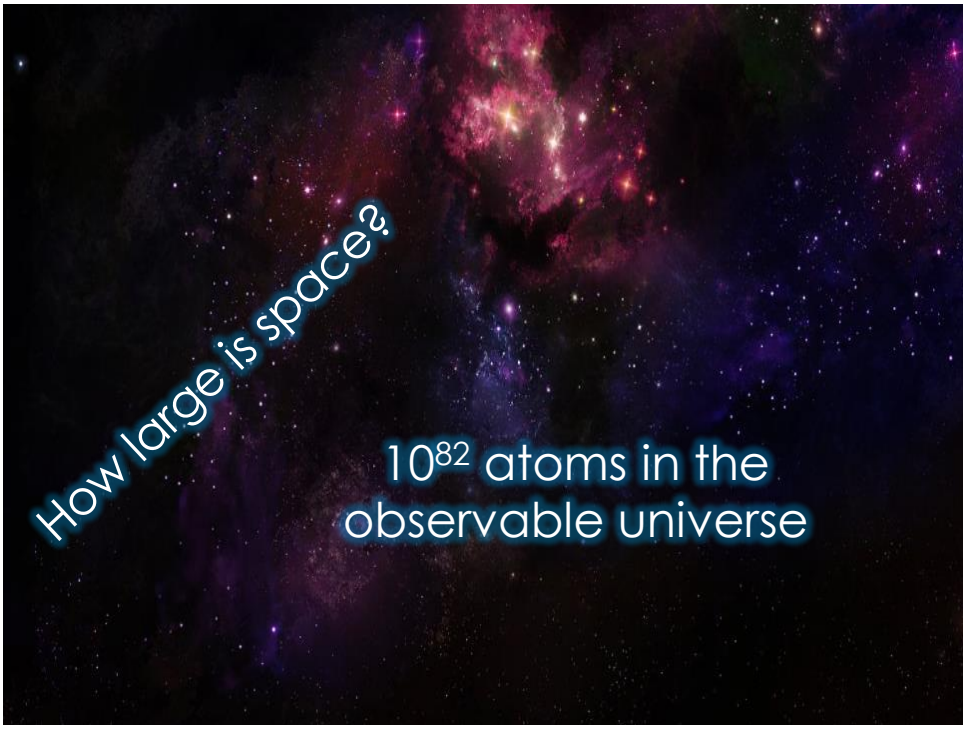
Clean Energy

Advanced drugs

Water purification



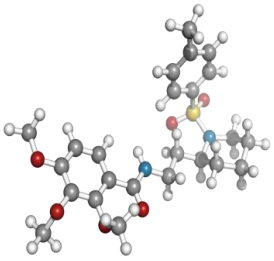
Molecules and materials



How large is chemical space?

10^{60} – 10^{180} medium-size molecules

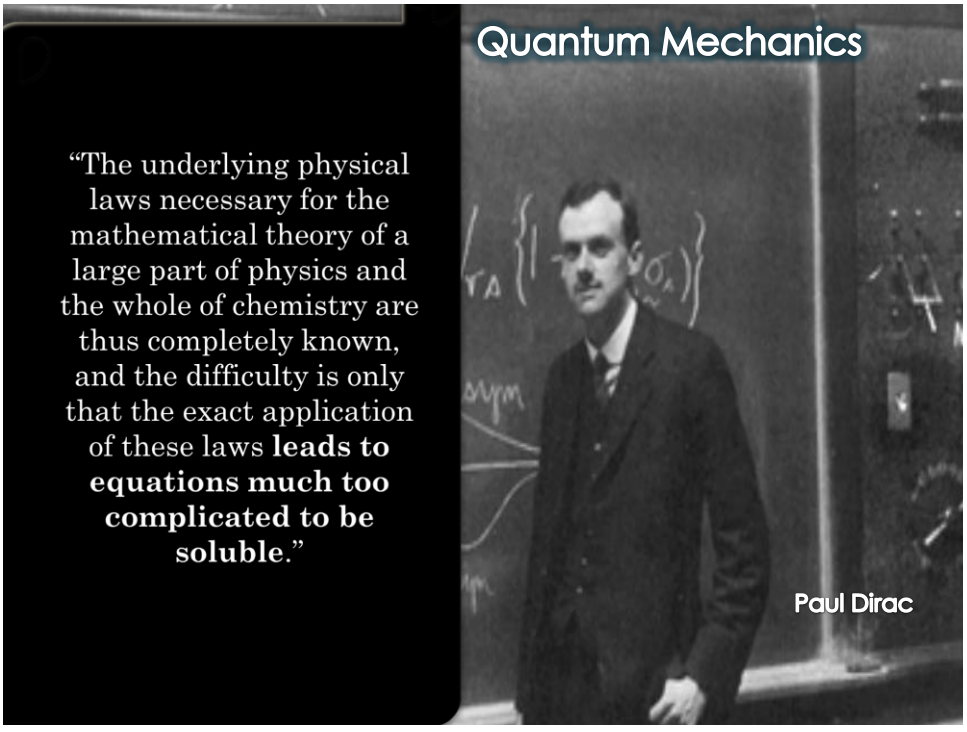
Molecular screening



Quantum Mechanics

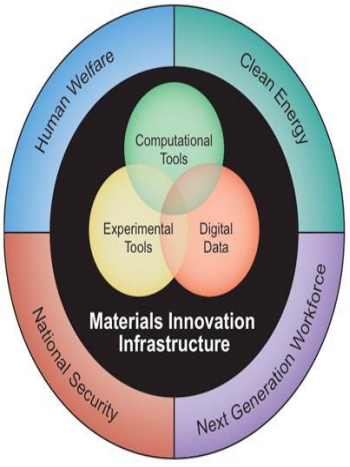
Machine Learning

How good is this molecule as a solar cell material?

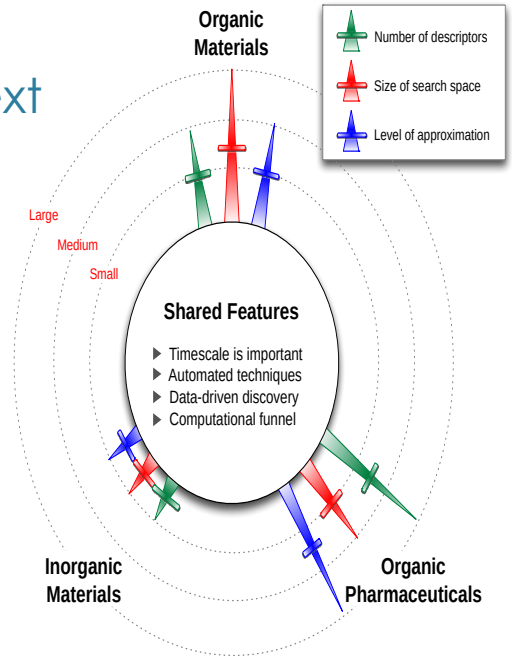

Quantum Mechanics
"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws **leads to equations much too complicated to be soluble.**"
Paul Dirac


" A breakthrough in machine learning would be worth ten Microsofts"
Bill Gates

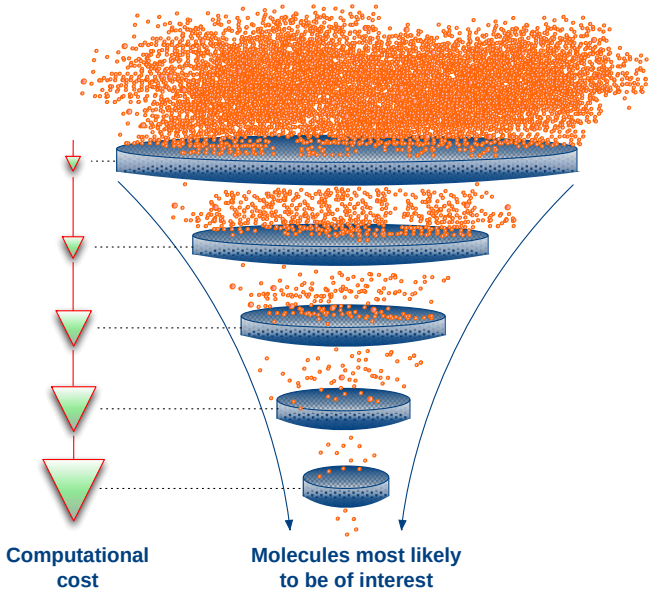
Organic materials in the larger context



US Materials Genome Initiative



From 10^{60} to 10^{6} to 10...



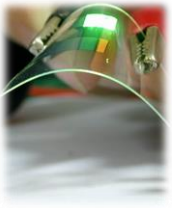
Initial library

Computational screening

Synthesis and testing

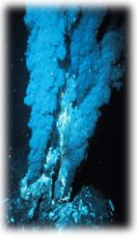
My research group's explorations of chemical space

The Harvard Clean Energy Project
Generating renewable energy



Blue Organic LED
For your next gadget or TV

Organic flow batteries
Storing renewable energy



Origins of life
How life may have come about?

The Harvard Clean Energy Project

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Generating renewable energy

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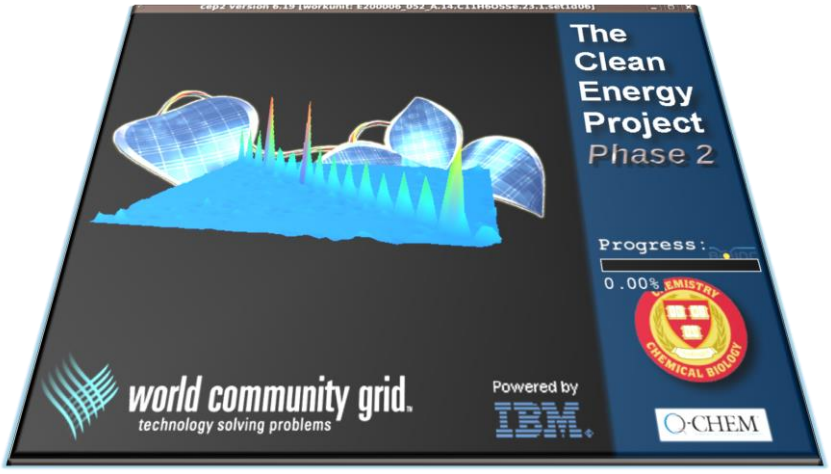
Origins of life
How life may have come about?

Power for 1.4 billion

Sheila Kennedy, MIT

How does an organic solar cell work?

Idle computers to the rescue!

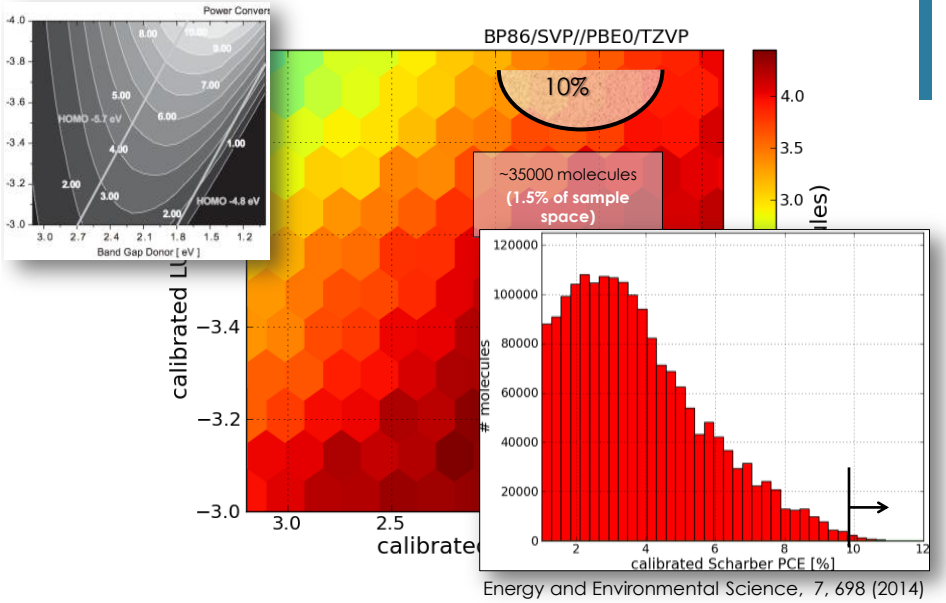


30,000 CPU years
25,000 molecules /day

35 million conformers
500 million quantum calculations

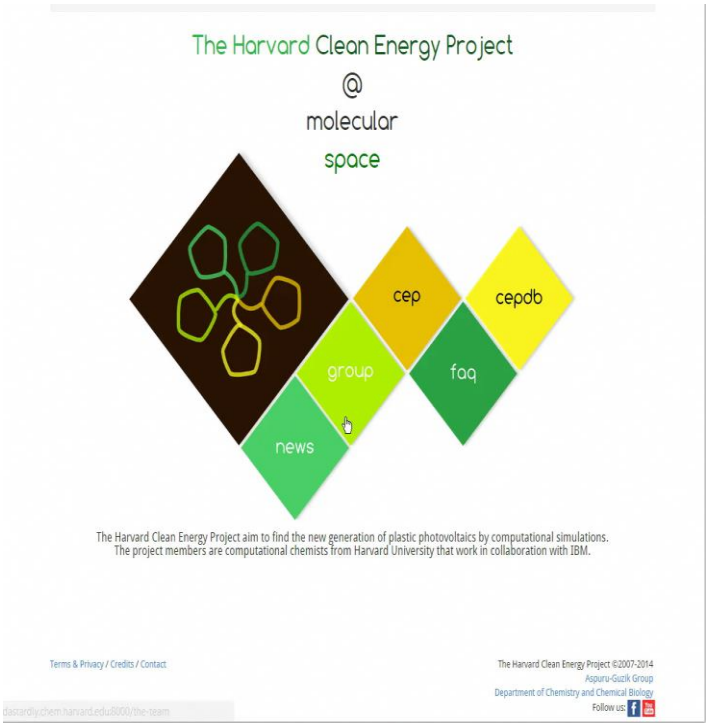
Largest quantum chemistry survey carried out to date

Sifting through 2.3 million molecules



Energy and Environmental Science, 7, 698 (2014)

Clean Energy Project Database



Organic Flow Batteries

The Harvard Clean Energy Project
Generating renewable energy

Blue Organic LED
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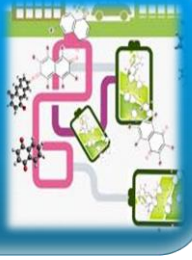
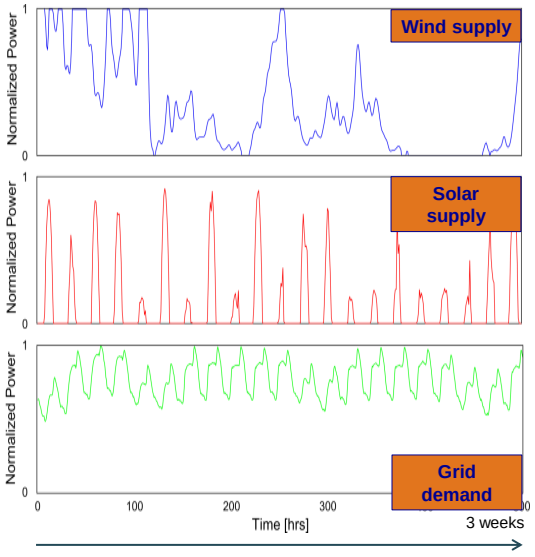
Organic flow batteries
Storing renewable energy



Origins of life
How life may have come about?

Renewables are intermittent



J. Rugolo and M.J. Aziz, *Energy Environ. Sci.* 5, 7151 (2012)

What is a flow battery?

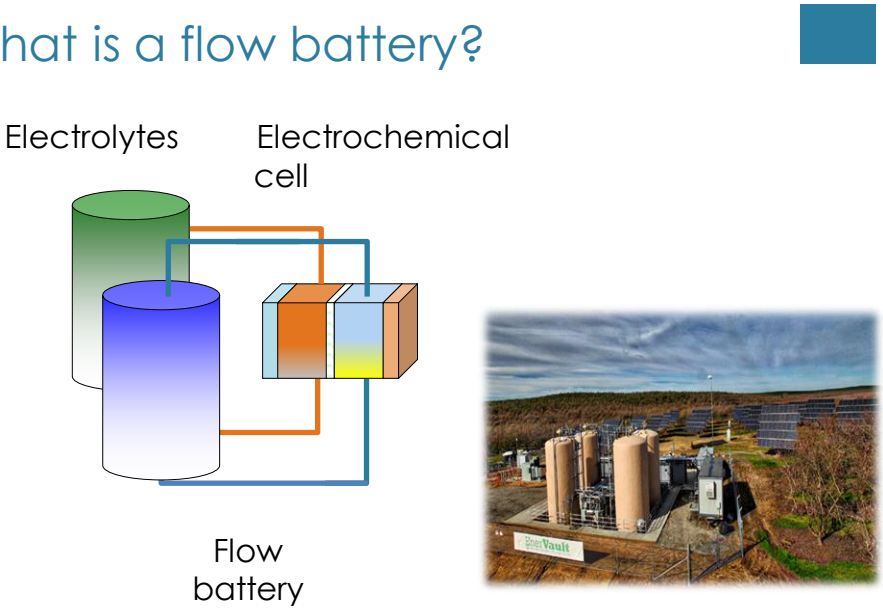
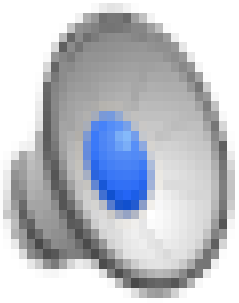


Image source: Enervault

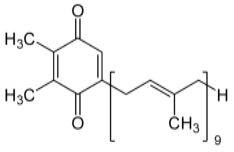


Vanadium flow battery

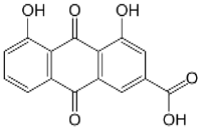
Metal free? Organic molecules?

Meet the quinones

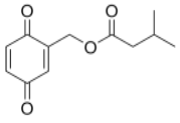
Plastoquinone:
Electron shuttle in plants



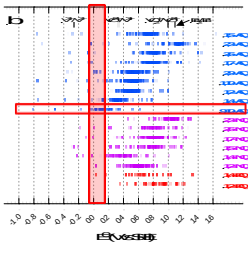
Rhein from Rhubarb:
is a **laxative**
and **antibacterial**

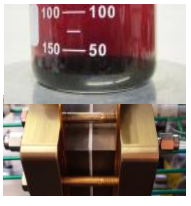


Blattellaquinone: is a sex **pheromone** female cockroaches use to attract males



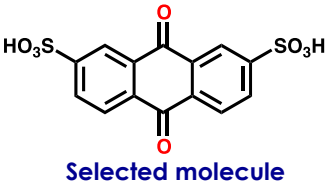
Our metal-free aqueous flow battery





Computational screening of
10,000 quinone molecules

Synthesize molecules
Test in flow battery



Selected molecule

Theory-experiment collaboration

LETTER

doi:10.1038/nature12909

A metal-free organic–inorganic aqueous flow battery

Brian Huskinson[1]*, Michael P. Marshak[1,2]*, Changwon Suh[2], Süleyman Er[2,3], Michael R. Gerhardt[1], Cooper J. Galvin[2], Xudong Chen[2], Alán Aspuru-Guzik[2], Roy G. Gordon[1,2] & Michael J. Aziz[1]

Michael Aziz
Engineering

Roy Gordon
Chemistry

Alán Aspuru-Guzik
Chemistry

Nature, 505, 2014, p. 195

Molecular Flow Battery Data View

Blue: Stable molecule
Red: Unstable molecule

X axis: Redox Potential
Y axis: Free energy of Solvation

~ 100,000 molecules shown

Molecular Flow Battery Data View

Filtering the data view

Molecular Flow Battery Data View

Baseball card view

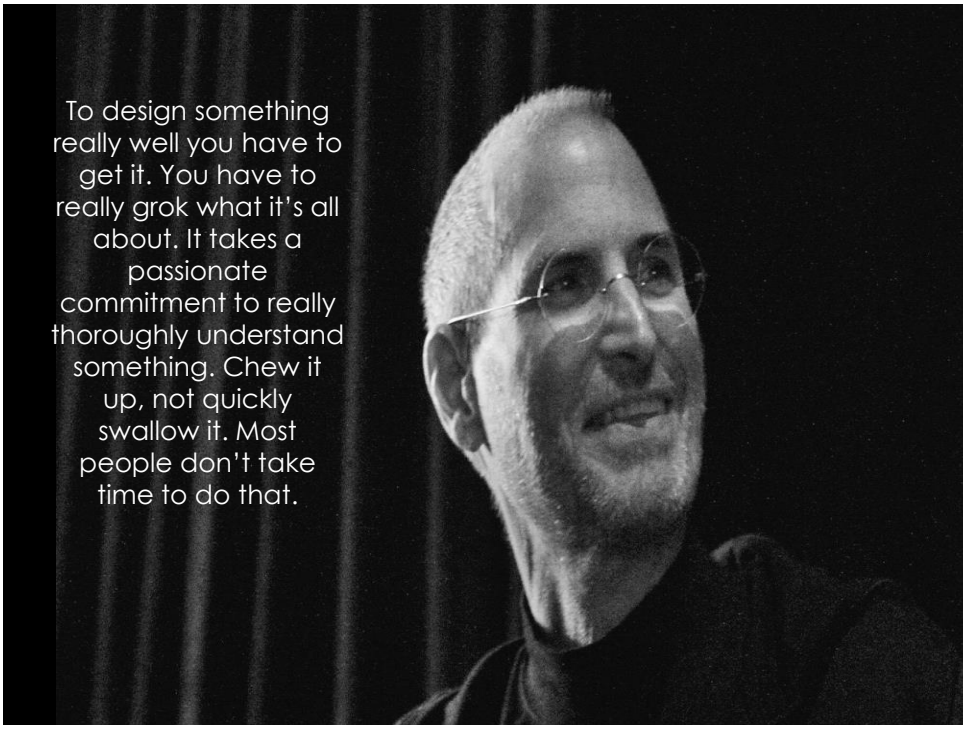
Molecular Flow Battery Data View

Redox pathways view

Selecting molecules is like dating.

Organic LED Screening

Synthetizability voting tool



DOE, ARPA-E, NSF, Samsung, Sloan Foundation
Camille and Henry Dreyfus Foundation

References

Clean Energy Project
J. Phys. Chem. Lett. 2, 2241 (2011)
Energy Environ. Sci. 4, 4849 (2011)
Energy Environ Sci 7, 698 (2014)
Organic Flow Battery
Nature 505, 195 (2014)
Chemical Science. Advance (2014)

Origins of life
J Comp
Theo Chem 10, 2097 (201

Organic electronics
Nat. Comm. 2, 437 (2011)
Nature 480, 504 (2011)

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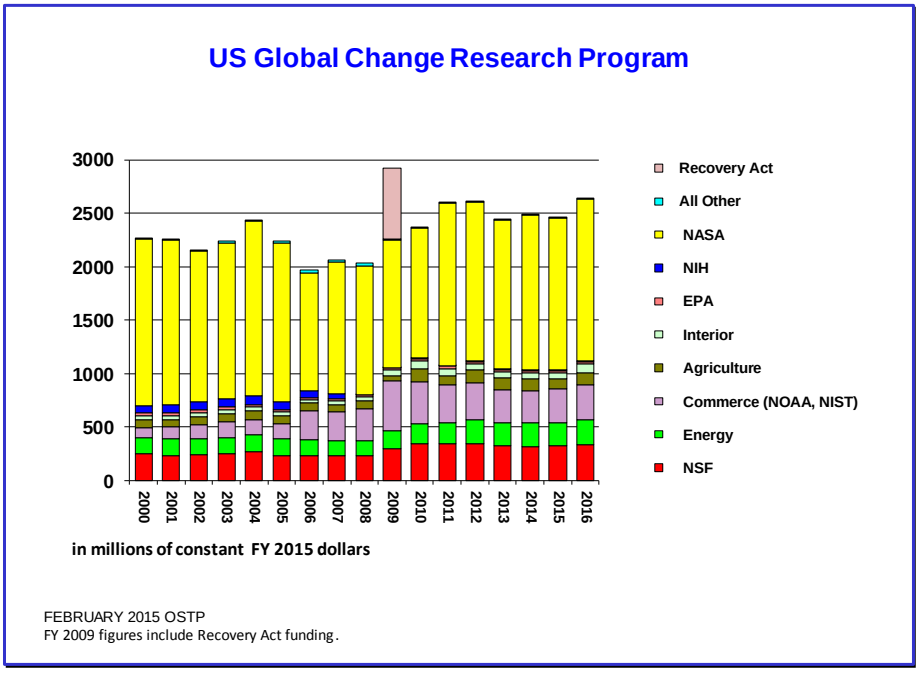
***Donna Cox**, National Center for Supercomputing Applications*
The Art of Visualizing Big Data

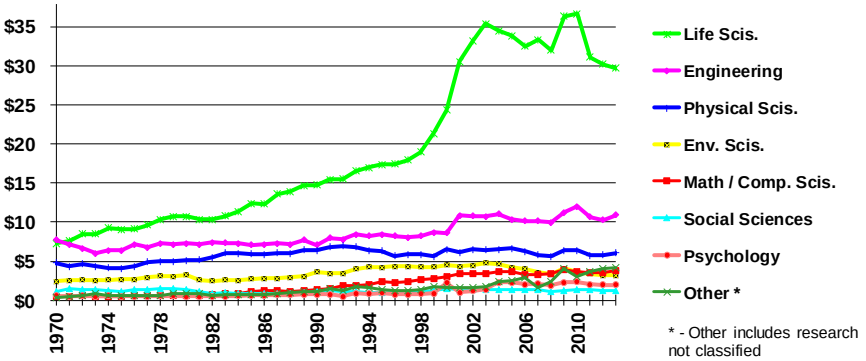
Utilizing Visual Insights in Science and Technology Policymaking

- **Kei Koizumi**
- **AAAS Annual Meeting February 2015**
- **For the session Visualization Insights from Big Data: Envisioning Science, Engineering, and Innovation**



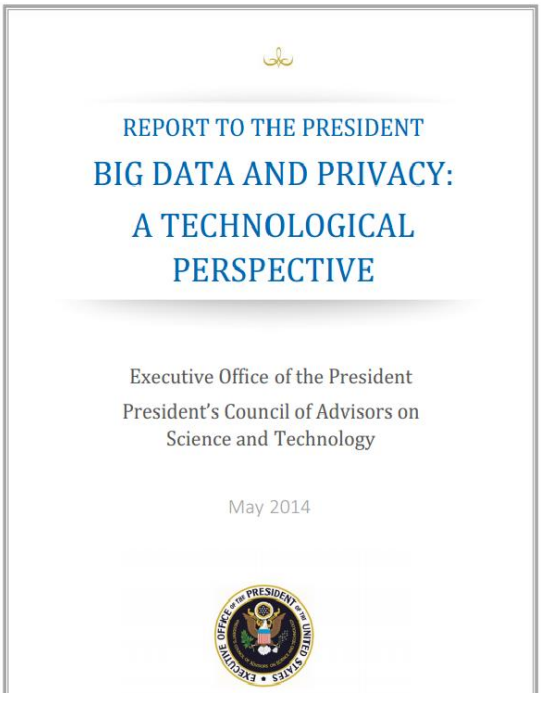
Trends in Federal Research by Discipline, FY 1970-2013

obligations in billions of constant FY 2014 dollars



* - Other includes research not classified (includes basic research and applied research; excludes development and R&D facilities)

Source: NSF, Survey of Federal Funds for Research and Development, 2013. FY 2012 and 2013 data are preliminary. Constant-dollar conversions based on OMB's GDP deflators. FY 2009 and 2010 include Recovery Act obligations.
DECEMBER 2013 OSTP



REPORT TO THE PRESIDENT

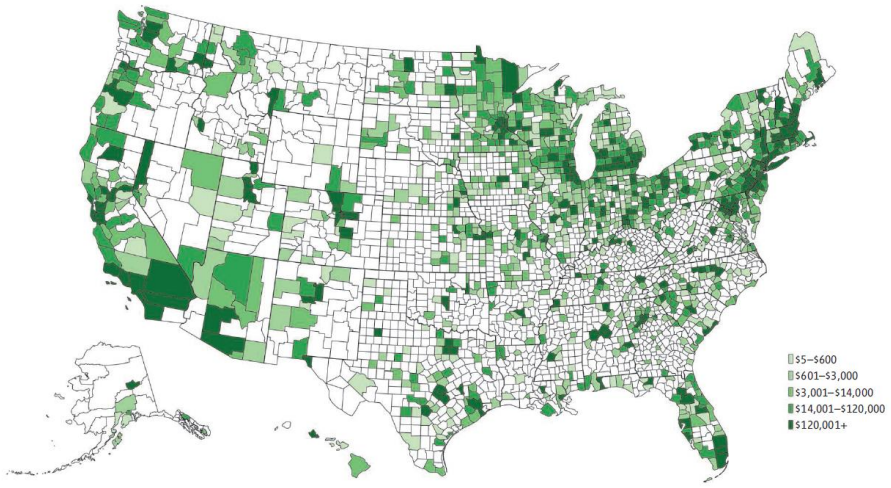
BIG DATA AND PRIVACY:

A TECHNOLOGICAL PERSPECTIVE

Executive Office of the President

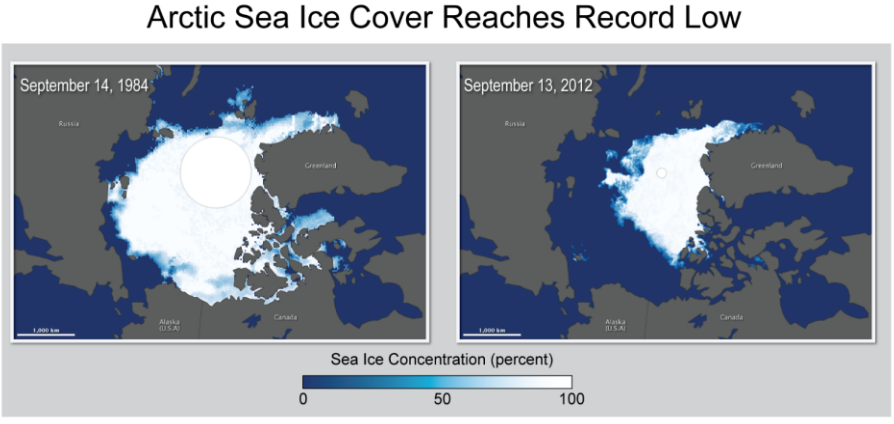
President's Council of Advisors on Science and Technology

May 2014

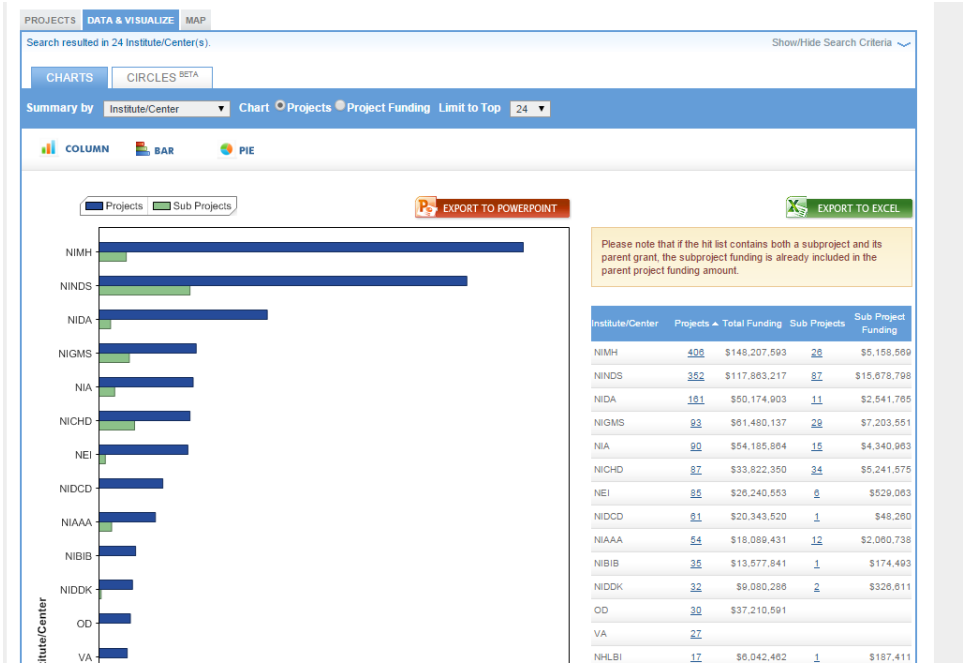


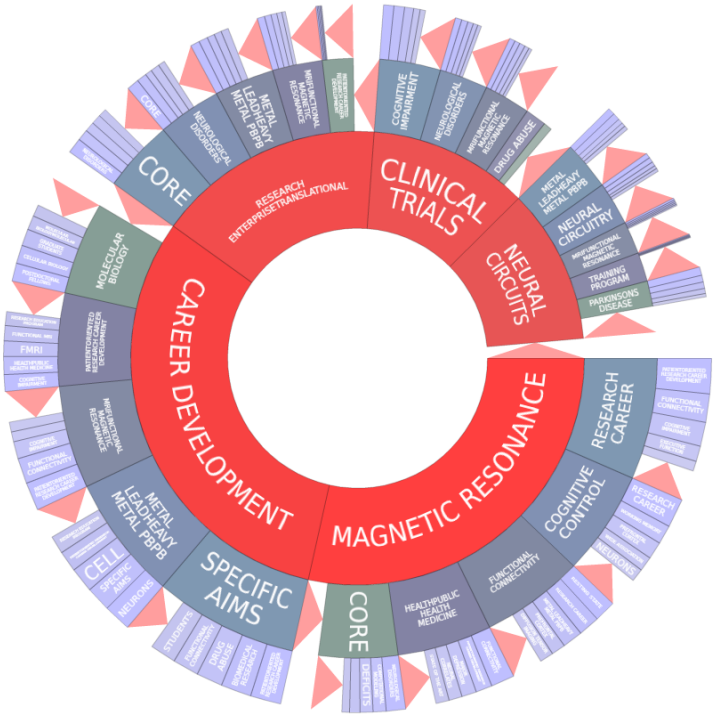
The geographic distribution of vendor and subaward expenditures. (See SM.)

Science Funding and Short-Term Economic Activity,
Bruce A. Weinberg, Jason Owen-Smith, Rebecca Rosen, Lou Schwarz, Barbara McFadden Allen, Roy Weiss, Julia Lane. Published 4 April 2014, *Science* 343, 41 (2014)

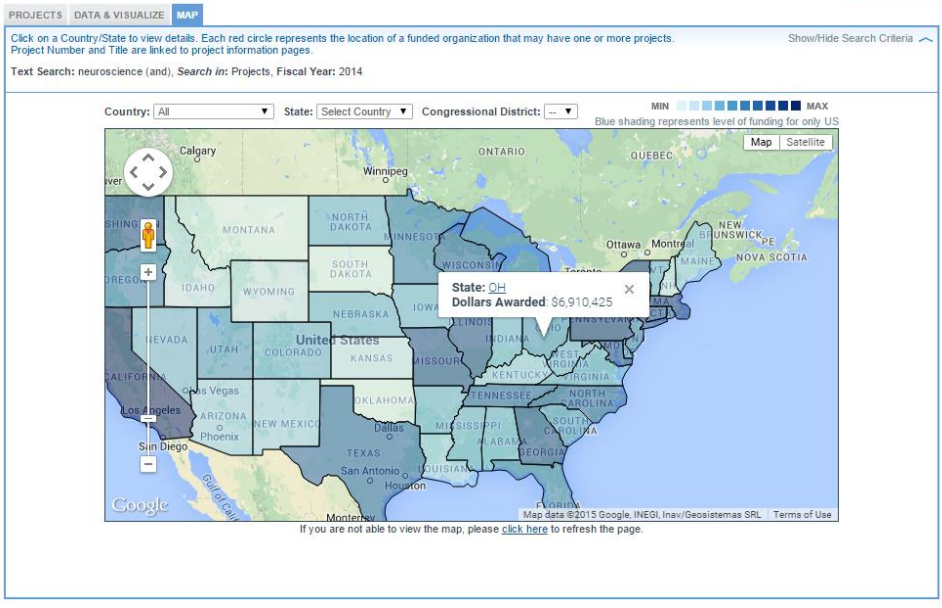


NASA Earth Observatory, EOS Project Science Office, NASA Goddard Space Flight Center
Visualizing the 2012 Sea Ice Minimum
URL http://earthobservatory.nasa.gov/IOTD/view.php?id=79256
2012


PROJECTS
DATA & VISUALIZE
MAP
Search resulted in 24 Institute/Center(s).
Show/Hide Search Criteria
CHARTS
CIRCLES BETA
Summary by Institute/Center
Chart Projects Project Funding
Limit to Top 24
COLUMN
BAR
PIE
Projects
Sub Projects
EXPORT TO POWERPOINT
EXPORT TO EXCEL
NIMH
NINDS
NIDA
NIGMS
NIA
NICHD
NEI
NIDCD
NIAAA
NIBIB
NIDDK
OD
VA
Please note that if the hit list contains both a subproject and its parent grant, the subproject funding is already included in the parent project funding amount.
Institute/Center
Projects
Total Funding
Sub Projects
Sub Project Funding
NIMH 406 $148,207,593 28 $5,158,569
NINDS 352 $117,863,217 87 $15,678,798
NIDA 161 $50,174,903 11 $2,541,765
NIGMS 93 $61,480,137 28 $7,203,551
NIA 90 $54,185,864 15 $4,340,963
NICHD 87 $33,822,350 34 $5,241,575
NEI 86 $26,240,553 6 $529,063
NIDCD 81 $20,343,520 1 $48,260
NIAAA 54 $18,089,431 12 $2,060,738
NIBIB 35 $13,577,841 1 $174,493
NIDDK 32 $9,080,286 2 $326,611
OD 30 $37,210,591
VA 27
NHLBI 17 $6,042,462 1 $187,411


CAREER DEVELOPMENT
CLINICAL TRIALS
MAGNETIC RESONANCE
NEURAL CIRCUITS
RESEARCH CAREER
SPECIFIC AIMS
CORE
RESEARCH ENTERPRISETRANSLATIONAL
MOLECULAR BIOLOGY
COGNITIVE CONTROL
NEURAL CIRCUITRY
COGNITIVE IMPAIRMENT
NEUROLOGICAL DISORDERS
DRUG ABUSE
METAL LEADHEAVY METAL PBPB
FUNCTIONAL CONNECTIVITY
TRAINING PROGRAM
PARKINSONS DISEASE
FMRI
CELL

1S10OD018448-01	3T MRI SCANNER FOR MULTIDISCIPLINARY IMAGING AND IMAGE-GUIDED THERAPY
1R01AT008225-01	MRCT EFFECTS ON BRAIN MECHANISMS OF INTEROCEPTIVE AWARENESS AND RUMINATION IN MDD
3R01MH101514-02S1	USING CBT TO EXAMINE CIRCUITRY OF FRUSTRATIVE NON-REWARD IN AGGRESSIVE CHILDREN
1I01RX001155-01A1	MOBILE SIGNAL PROCESSING SYSTEM FOR BROADBAND NEURAL DECODING
1U54NS092091-01	CLINICAL RESEARCH IN ALS & RELATED DISORDERS FOR THERAPEUTIC DEVELOPMENT (CIRCATE)
1R01MH105246-01	OPTIMIZING COGNITIVE TRAINING TO IMPROVE FUNCTIONAL OUTCOME IN CLINICAL HIGH RISK
1R25OD016516-01	A PARTNERSHIP IN NEUROSCIENCE EDUCATION
1K23HD074736-01A1	MULTIMODAL EVALUATION OF SENSORY PROCESSING AND NEURODEVELOPMENT IN NICU INFANTS
5T32MH093315-03	POSTDOCTORAL TRAINING IN REPRODUCTIVE MOOD DISORDERS
5U24DK097771-02	NIDDK NETWORK COORDINATING UNIT
5P30MH075673-09	CENTER FOR NOVEL THERAPEUTICS FOR HIV-ASSOCIATED COGNITIVE DISORDERS
5R13CA086959-14	THE ANNUAL BLOOD-BRAIN BARRIER CONSORTIUM MEETING
3U01AG024904-09S3	ALZHEIMER'S DISEASE NEUROIMAGING INITIATIVE
1R01NR015223-01A1	INTERVENTIONS FOR SYMPTOM MANAGEMENT IN OLDER PATIENTS WITH HAND
5P50DA018165-08 (0481)	EDUCATION CORE
5U10NS077423-04	UNIVERSITY OF MIAMI: NETWORK OF EXCELLENCE INNEUROSCIENCE CLINICAL TRIALS (NEXT)
5U10NS077382-04	NETWORK OF EXCELLENCE IN NEUROSCIENCE CLINICAL TRIAL CENTER AT THE OHIO STATE UNI
5P50MH100029-03	MECHANISMS OF RISK AND RESILIENCE IN ASD: ONTOGENY, PHYLOGENY AND GENE DISRUPTION
5K01HD069504-04	BRAIN STIMULATION- AIDED STROKE REHABILITATION: NEURAL MECHANISMS OF RECOVERY
5T32EY023211-02	TRANSLATIONAL VISION SCIENCE RESEARCH AT OREGON HEALTH & SCIENCE UNIVERSITY
1R01MH104423-01	MOBILIZING COMMUNITY SYSTEMS TO ENGAGE FAMILIES IN EARLY ASD DETECTION & SERVICES
5T32NS007338-25	EXPERIMENTAL THERAPEUTICS IN NEUROLOGICAL DISEASE
5U10NS077311-04	CINCINNATI NEUROSCIENCE CLINICAL TRIALS RESEARCH CENTER (CINCINEXT)




CLIMATE EXPLORER
LAYERS
HISTORICAL DATA
TOPICS:
Ecosystem Vulnerability
Climate Stressors
Current Drought
Drought (9/24/2013)
People and Assets Impacted
Population Density (2000)
Land Cover (2011)
Weekly VCI (9/24/2013)
LAYER INFORMATION
San Francisco


CLIMATE EXPLORER
LAYERS
HISTORICAL DATA
TOPICS:
Coastal Flood Risk
Climate Stressors
Inundation from Sea Level Rise (1ft)
Inundation from Sea Level Rise (2ft)
Inundation from Sea Level Rise (3ft)
People and Assets Impacted
Population Density (2000)
Coastal Vulnerability to Sea Level Rise
Social Vulnerability Index
LAYER INFORMATION
Inundation from Sea Level Rise (2ft)
Source: NOAA Coastal Services Center
Extent and relative depth of high-tide flooding after 2 feet of sea level rise.
Hayward
Fremont
Modesto
Sunnyvale
Santa Clara
San Jose

Thank you

Kei Koizumi

Disclaimer: The views expressed here are my own and do not represent the views of the Office of Science and Technology Policy or any other organization.

Visualization Insights from Big Data: Envisioning Science, Engineering, and Innovation

Friday, 13 February 2015: 8:00 AM-9:30 AM
Room LL20D (San Jose Convention Center)

Advanced data mining and visualization techniques can be used to extract patterns and trends from large and complex datasets. Resulting visualizations help manage, navigate, and understand vast amounts of information; support new discoveries and questions; and are a great tool to communicate science to a general audience. This interdisciplinary session brings together experts from chemistry, engineering, science policy, and art to showcase visual solutions that are instrumental in achieving high return on investment; science mapmakers who use visual analytics to identify emerging areas of research and innovation, calculate the impact of science policy interventions, and predict science and technology trends; and visual techniques that render the abstract into the concrete using computer graphics and cinematic approaches. This session will be extremely visual to highlight novel information mining and imaging techniques that enhance understanding and improve daily decision-making.

Organizer: *Katy Borner, Indiana University*

Co-Organizer: *Joseph E. Sabol, Chemical Consultant*

Speakers:

***Alan Aspuru-Guzik**, Harvard University*
Billions and Billions of Molecules: Exploring Chemical Space for New Energy Materials

***Kei Koizumi**, U.S. Office of Science and Technology Policy*
Utilizing Visual Insights in Science and Technology Policymaking

***Donna Cox**, National Center for Supercomputing Applications*
The Art of Visualizing Big Data

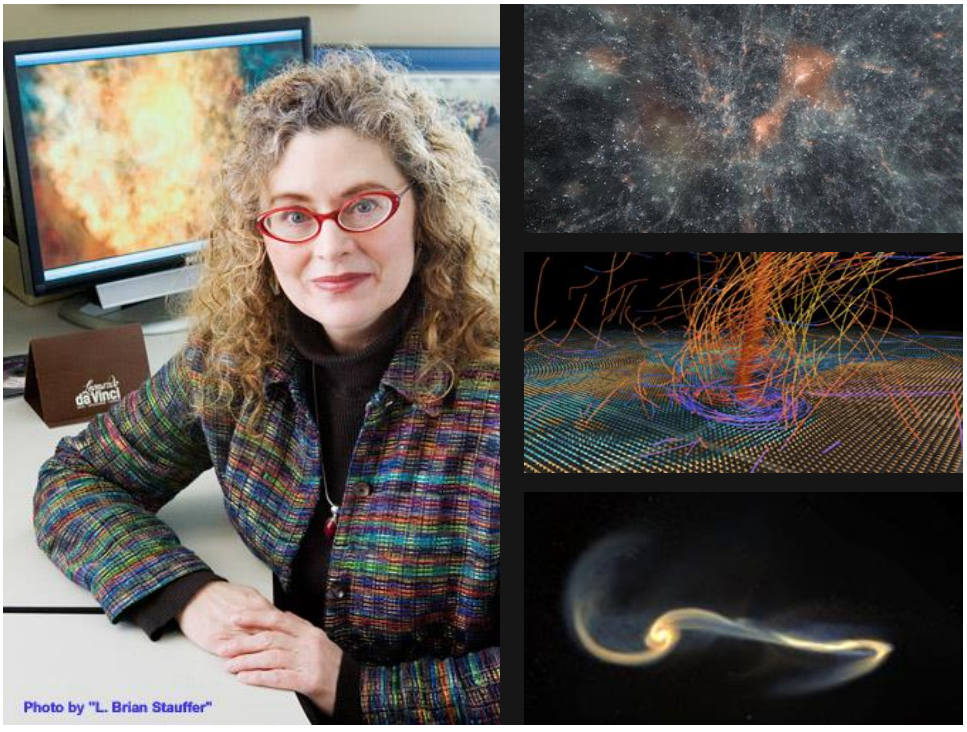
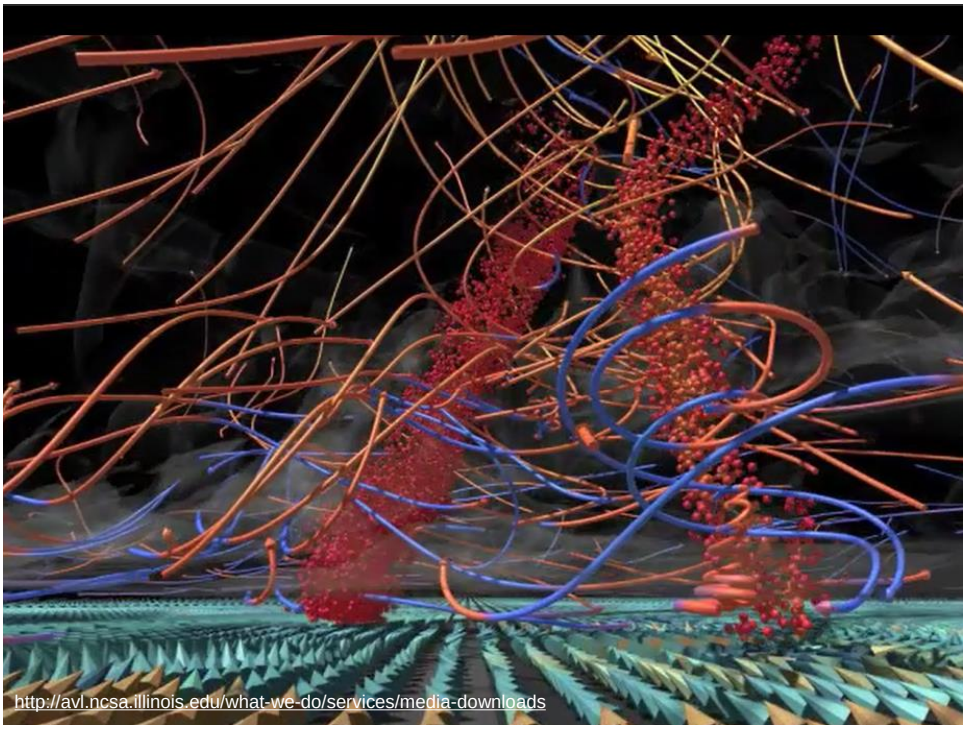
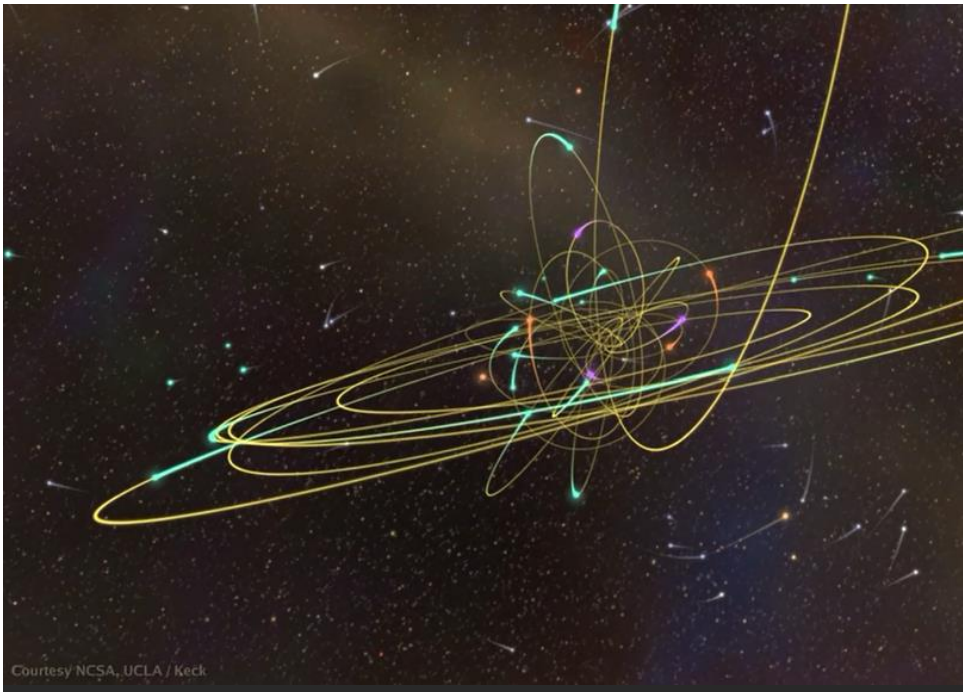


Photo by "L. Brian Stauffer"


http://avl.ncsa.illinois.edu/what-we-do/services/media-downloads

http://avl.ncsa.illinois.edu/what-we-do/services/media-downloads

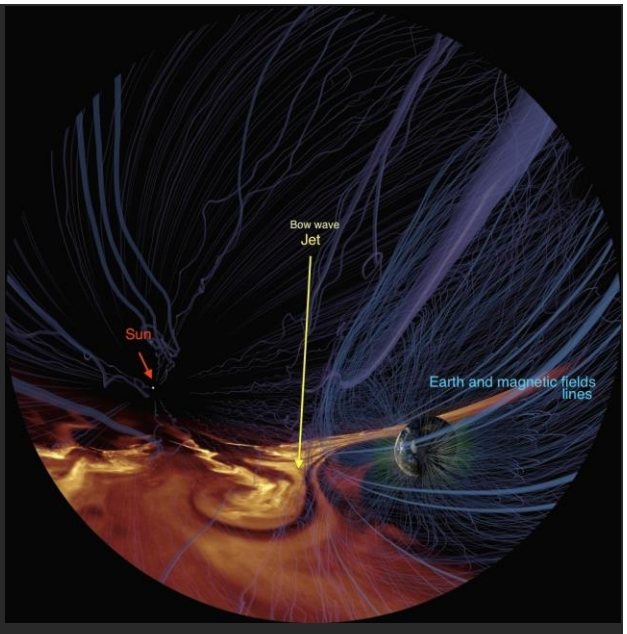


http://avl.ncsa.illinois.edu/what-we-do/services/media-downloads

Still from the new full dome show “Solar Superstorms.”

Visualization of scientific numerical model reveals a turbulent front generated by a solar wind interacting with Earth’s magnetic field during a powerful solar storm.

Large disturbances, including high velocity jets, can penetrate deep inside the Earth’s magneto-sphere and result in space weather effects such as loss of communications satellites and wide spread blackouts.



Numerical simulation by Homa Karimabadi, Mahidhar Tatineni and Vadim Roytershteyn, University of California, San Diego. Visualization by the Advanced Visualization Lab (Donna Cox, Robert Patterson, Stuart Levy, AJ Christensen, Kalina Borkiewicz, Jeff Carpenter) at NCSA. Funded in part by the National Science Foundation.

12–16 FEBRUARY **AAAS 2015 ANNUAL MEETING** SAN JOSE, CA
INNOVATIONS, INFORMATION, AND IMAGING

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Q&A

***Kei Koizumi**, U.S. Office of Science and Technology Policy*
Utilizing Visual Insights in Science and Technology Policymaking

***Donna Cox**, National Center for Supercomputing Applications*
The Art of Visualizing Big Data

Places & Spaces: Mapping Science

Sunday, 15 February 2015
Exhibit Hall (San Jose Convention Center)

***Katy Börner** , Indiana University, Bloomington, IN*
Todd N. Theriault , Indiana University, Bloomington, IN
Elizabeth G. Record , Indiana University, Bloomington, IN

Background: The *Places & Spaces: Mapping Science* exhibit was developed to introduce visualizations of the evolving science and technology (S&T) 'landscape' to a general audience. The maps show the structure and interconnections between scientific disciplines, the birth of new 'lands' of science, and the diffusion of ideas across the landscape of science. Each iteration showcases the benefits of data visualization for a particular audience, e.g., for economic decision makers, science policy makers, scholars, librarians, and kids. At its heart, the exhibit's goal is to promote validated and replicable workflows for the design of data visualization and to increase public understanding of the power of S&T maps to help us accurately make sense of the increasingly large streams of scientific data that we all face on a daily basis. **Methods:** *Places & Spaces* debuted in 2005 and was conceived as a ten-year project. Each year, a themed call for maps is issued and a team of international reviewers and exhibit advisors selects the most insightful and innovative maps submitted. The top-10 maps are reworked for public display at libraries, science museums, and national science academies, and then the high-resolution 30" x 24" maps are printed, laminated, and framed. In its tenth year, the exhibit now includes 100 maps, featuring the best examples of knowledge domain mapping, novel location-based cartographies, data visualizations, and science-inspired art works.

INTELLECTUAL PROPERTY & SCIENCE

THOMSON REUTERS

JOIN US: AAAS LUNCHEON DISCUSSION

VISUALIZATION METAPHORS FOR COMMUNICATING THE STRUCTURE AND DYNAMICS OF SCIENCE

JULIA LAURIN, THOMSON REUTERS AND KATY BÖRNER, INDIANA UNIVERSITY

Please join us and take part in our lunchtime discussion titled "Visualization Metaphors for Communicating the Structure and Dynamics of Science" hosted by Julia Laurin, Thomson Reuters and Katy Börner, Indiana University.

Date: Sunday, February 15, 2015

Time: 12 PM to 1 PM (PST)

Location: San Jose Convention Center
AAAS Conference Room: Glen Ellen
150 West San Carlos Street
San Jose, CA 95113

This luncheon will provide an opportunity for those who produce and work with maps of science to discuss the challenges of visualizing non-spatial scientific activity and investigate concrete ways for scholars and industry to advance understanding and engagement with maps of science. Brief talks by leading experts and brainstorming will be used to identify: What visual metaphors have been successful for representing trends, emerging research areas, or bursts of activity, etc.? Are there best practices for representing non-spatial information? How can the different teams producing maps of science collectively enhance the legibility and utility of science maps?

Humanexus

Watch the official trailer »

Producer/Script Writer: Katy Börner, Designer/Artist: Ying-Fang Shen, Sound Artist: Norbert Herber, 2013.
http://cns.iu.edu/humanexus