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 Börner, 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

- **Kel 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
Map of Scientific Collaborations from 2005-2009

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

The Structure of Science

The Structure of Science - Kevin Boyack, Richard Klavans - 2005
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 “Expediton 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](http://www.expedition-zukunft.de)
References


Billions and Billions of Molecules

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

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

Exploring Chemical Space for Energy Materials
Some of the challenges of the 21st century

Clean Energy

Advanced drugs

Water purification

Molecules and materials

How large is space?

$10^{82}$ atoms in the observable universe
How large is chemical space?

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

Molecular screening

How good is this molecule as a solar cell material?

Quantum Mechanics

Machine Learning
"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
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?
Power for 1.4 billion

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)
Organic Flow Batteries

The Harvard Clean Energy Project
Generating renewable energy

Blue Organic LED
For your next gadget or TV

Origins of life
How life may have come about?
Renewables are intermittent

What is a flow battery?

Electrolytes → Electrochemical cell

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

Michael Aziz
Engineering

Roy Gordon
Chemistry

Alán Aspuru-Guzik
Chemistry

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
Selecting molecules is like dating.
Organic LED Screening

Synthetizability voting tool

To design something really well you have to get it. You have to really grok what it’s all about. It takes a passionate commitment to really thoroughly understand something. Chew it up, not quickly swallow it. Most people don’t take time to do that.
References

Clean Energy Project
Energy Environ. Sci. 4, 4849 (2011)

Organic Flow Battery
Nature 505, 195 (2014)
Chemical Science.
Advance (2014)

Origins of life
J Comp Theo Chem 10, 2097 (2014)

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

In millions of constant FY 2015 dollars

FEBRUARY 2015 OSTP
FY 2009 figures include Recovery Act funding.

* Other includes research not classified (includes basic research and applied research; excludes development and R&D facilities)
Science Funding and Short-Term Economic Activity,
Bruce A. Weinberg, Jason Owen-Smith, Rebecca Rosen, Lou Schweitzer, Barbara
McFadden Allen, Roy Weiss, Julia Lane. Published 4 April 2014, Science 343, 41 (2014)

Arctic Sea Ice Cover Reaches Record Low

NASA Earth Observatory, EOS Project Science Office, NASA Goddard Space Flight Center
Visualizing the 2012 Sea Ice Minimum
URL http://earthobservatory.nasa.gov/IOY/view.php?id=79296
2012
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.
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, Al Christensen, Kalina Borkiewicz, Jeff Carpenter) at NCSA. Funded in part by the National Science Foundation.

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

Friday, 13 February 2015: 8:00 AM-9:30 AM
Room LL203 (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 Borer, 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
Plances & 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 calls 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.

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 further the development of new and better ways to communicate the structure and dynamics of science. The discussion will also 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

http://cns.iu.edu/humanexus