

Modelling Science, Technology, Innovation

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Abstract

In a knowledge-based economy, science and technology are omnipresent and their importance is undisputed. Equally evident is the need to allocate resources, both monetary and human, in an effective way to foster innovation (Ahrweiler et al., 2015; Watts & Nigel, 2014). In the preceding decades, science policy has embraced data mining and metrics to gain insights into the structure and evolution of science and to devise metrics and indicators (Hicks et al., 2015), but it has not invested significant efforts into mathematical, statistical and computational models that can predict future developments in science, technology, and innovation (STI) despite their power. STI models make it possible to simulate the diffusion of ideas and experts, to estimate the impact of population explosion and aging, to explore alternative funding schemas, or to communicate the probable outcomes of different policy decisions.

Advances in computational power combined with the unprecedented volume and variety of data on science and technology developments (e.g., publications, patents, funding, clinical trials, stock market, social media data), create ideal conditions for the advancement of computational modeling approaches that can be empirically validated and used to simulate and understand the structure and dynamics of STI and to augment human decision making.

An NSF-funded conference “Modelling Science, Technology, and Innovation” was held at the National Academy of Sciences Building in Washington DC in May 2016. More than 100 participants from 67 institutions and seven countries attended the conference; 62 experts from academia, government, and industry presented their work. This paper provides a brief introduction into mathematical, statistical, and computational STI models and then highlights key challenges, insights, and opportunities associated with their usage in decision making as well as key insights that resulted from the conference. The full conference report together with all presentation slides and recordings is available at <http://modsti.cns.iu.edu>.

Introduction

Models of science, technology, and innovation (STI) aim to inform (policy) decision making in education, energy, healthcare, security and other sectors (Börner, 2016). They do not replace but empower experts to make informed decisions when selecting reviewers, picking the best proposals for funding, or when making resource allocation decisions. They are a new kind of “macroscopic tool” (de Rosnay, 1979) that

help derive key insights from big data in support of evidence-based policy. As Kevin Finneran, National Academies of Sciences, Engineering, and Medicine noted in his presentation: “If retail has figured out how to optimize sales by using models, then there is likely a market in government for practical decisions.”

Some models are optimized to make recommendations, e.g., IBM Watson suggesting reviewers for a set of proposals, without much information on the type of match or the matching process. Other models aim to capture the true structure and dynamics of complex STI systems; they simulate the diffusion of ideas and experts, estimate the impact of population explosion and aging, or communicate the probable outcomes of different policy decisions. In sum, they help answer resource allocation or multi-faceted strategic questions. The latter models are often used in a team setting where small multi-disciplinary groups investigate and debate alternative futures together.

Computational models are already well established and widely used in a number of fields such as meteorology to predict weather and storms; epidemiology to predict and prevent pandemics; and climate to predict future scenarios and set carbon prices. Industry also extensively uses computational models to optimize operations, management, production, distribution, and marketing. Early adopters of data-driven decision making (most notably, Target, Walmart, and Amazon) now dominate their sectors. Those who were slow to invest and then did so in isolated aspects of the organization (most notably Sears, Kmart, and Barnes & Noble) are heading towards bankruptcy.

Advances in computational power combined with the availability of relevant data (e.g., publications, patents, funding, clinical trials, stock market, social media) create ideal conditions for the implementation of computational modeling approaches that can be empirically validated and used to simulate and understand future developments within STI and to pick desirable futures. Interactive data visualizations that show probable futures in response to different (policy) decisions or external events can help stakeholders discuss model assumptions, design, and output. Ideally, stakeholders get to “drive the future before it is implemented” (Rouse, 2014, 2015); they can quickly explore different policy options and discard those that lead to unexpected, undesired consequences (Watts & Gilbert, 2014; Ahrweiler et al, 2015). However, designing effective interfaces that let different stakeholders communicate and explore different scenarios is non-trivial.

ModSTI Examples

The book *Models of Science Dynamics* (2012) provides a unique review of major model classes (from population dynamics models to complex network models) accessible to science policy researchers and practitioners. Two special issues in *Scientometrics* entitled *Modeling science: Studying the structure and dynamics of science* (2011) and *Simulating the Processes of Science, Technology, and Innovation* (2016) feature exemplary STI models. Here we discuss two STI models in more detail. Example 1 describes how teams in various fields have evolved over time and what it is they contribute to contemporary science. Example 2 proposes radical changes to the current funding system. Both of these models were

empirically validated and a high correlation was found between the simulated datasets and the structures and dynamics found in publication and funding data.

The Importance of Small Teams in the Big Science Era

Contemporary science is a collaborative effort within an intricate network of people, institutions, concepts, and technology. Many projects are of such complexity or scope that they require joint efforts of many individuals with diverse expertise, reaching team sizes of few hundreds. Furthermore, studies suggest that large interdisciplinary teams are more likely to produce high impact work.

Only 50 years ago, the situation was very different. Most papers were written by single authors and the largest co-author teams did not exceed ten members. How did this change in the production of knowledge occur? How do science teams form and what processes lead to their expansion? What makes a successful team?

Research team size distribution lies at the heart of our understanding of collaborative practices and research productivity. As Figure 1 shows, knowledge production today is qualitatively different from that of earlier times: “little science” performed by individuals or small groups of researchers is to a large part superseded by “big science” efforts by large teams that span disciplinary, institutional, and national boundaries.

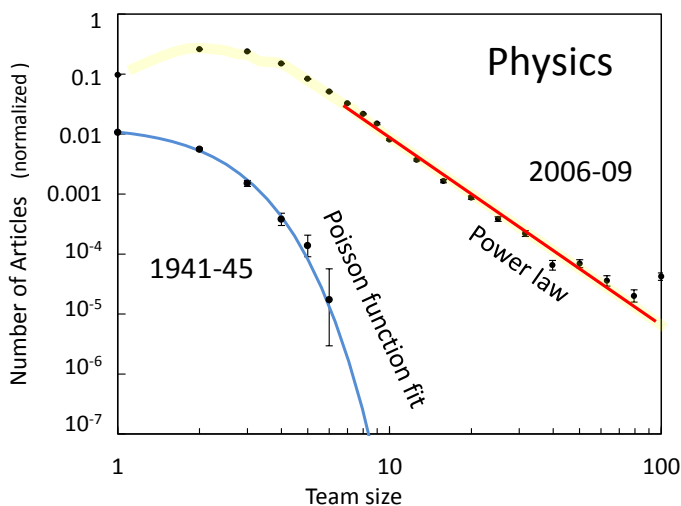


Figure 1. Change in the distribution of research team sizes in physics from a Poisson distribution to one dominated by a fat tail (a power law). In 1941-1945, for each paper with five authors, there were one thousand single-authored papers (blue). In 2006-2009, there are as many papers with five authors as there are single authored papers (red), and very large teams are not uncommon.

Staša Milojević at Indiana University developed a model of how teams emerge and grow, which accurately reproduces the change seen in Figure 1, and predicts how teams will evolve in the future. The model shows that team formation was, and remains, a Poisson process that results in relatively small, core teams (including single investigator teams) that are necessary to carry out certain types of research. The model also simulates the emergence of larger teams over the last 50 years in all fields of

science albeit with varying pace and magnitude of change. According to the model, each big team originates from a small team; while some small teams do not change in size, others quickly accumulate additional members proportionally to the past productivity of team members developing into big teams. Surprisingly, the model shows that relatively small teams dominate knowledge production in most fields, so that cumulatively they still contribute more new knowledge than large teams. These findings are of key importance to policy, because they show that increased funding emphasis on large teams may undermine the very process by which large, successful teams emerge.

Crowdsourcing Funding Allocation

Johan Bollen and colleagues at Indiana University argue that scholars “invest an extraordinary amount of time, energy and effort into the writing and reviewing of research proposals” plus funding agencies are consuming resources that could be more productively used to conduct and finance research. In a 2014 paper, they use NSF and Taulbee Survey data to provide a simple calculation of return on investment for scholars in computer science. The calculation quickly reveals that the return on investment is negative: Four professors working four weeks full-time on a proposal submission at labor costs of about \$35,000; given a CISE funding rate of 21% about five submission-review cycles might be needed, resulting in a total expected labor cost of \$175,000. The average NSF grant is \$164,526 per year of which U.S. universities charge about 50% overhead leaving about \$109,684 for research. That is, the four professors lose $\$175,000 - \$109,684 = \$65,316$ of paid research time by obtaining a grant and U.S. universities might like to forbid professors to apply for grants—if they can afford to forgo the indirect dollars. Note that this simple calculation does not cover any time spent by scholars to review proposals. In 2015 alone, NSF conducted 231,000 proposal reviews to evaluate 49,600 proposals.

Bollen et al. then go on to propose a FundRank model to (partially) replace the current process of government research funding allocation by expert-based crowdsourcing. In the new system, each eligible scholar (e.g., all eligible to submit NSF and NIH grants today) receives a certain dollar amount each year, let's say \$100,000. S/he then needs to give a certain fraction, e.g., 50%, to colleagues that are most deserving by logging into a centralized website and entering names and amounts. That is, scholars collectively assess each other's merit and they “fund-rank” other scholars, with highly ranking scholars receiving the most funding.

Instead of spending weeks writing and reviewing proposals, scholars are now incentivized to spend time communicating the value and impact of their past, current, and planned work so that others can judge their contributions. Using a fully digital system, conflicts of interest can be easily identified and honored; networks of mutual favors can be detected automatically, and results shared publicly.

FundRank was implemented using the recursive PageRank algorithm pioneered by Sergey Brin and Larry Page in 1998. Using PageRank, the “importance” (here reputation, value, impact) of a scholar depends not only on the number of scholars that vote for him/her but also their importance. The more important the scholars that link to a person, the more important the person must be. The FundRank model was validated using citation data from 37 million papers over 20 years as a proxy for how each scientist might distribute funds in the proposed system. Simulation results show funding patterns that have a

similar distribution compared to NSF and NIH funding for the past decade—at a fraction of the cost required by the current system.

ModSTI Challenges

There are diverse challenges associated with the usage of mathematical, statistical, and computational models of STI in decision making. The challenges are related to fundamental research, applied research, cyberinfrastructure, education, and outreach. Many of these challenges can be phrased as opportunities.

Fundamental Research

Research on STI is carried out by researchers in a wide range of disciplines: economics, social science, information science, science policy, scientometrics/bibliometrics, physics, and science policy among others that develop mathematical, statistical, and computational models of different types (stochastic, agent-based, epidemics, game-theoretic, network. etc.). One of the impeding factors in moving forward fundamental research is freely available access to good quality data that will reduce data curation efforts currently done by each individual team and to allow reproducibility (one of the most-wanted traits of models as identified by conference participants). Lack of obvious continuous sources for funding for this type of research was identified as an additional challenge.

In addition, researchers who do STI modeling publish in a wide range of venues, addressing different audiences. As became evident at the conference, current research efforts and results are not universally known to the researchers (let alone policy makers). Such a state slows the scientific progress and can possibly lead to unnecessary “reinvention of the wheel.” Conference participants genuinely enjoyed being in a truly intellectually diverse environment, which helped them shed new light to the problems they were grappling with, but also forced them to think and talk about their own research in a new way. There was a sense that similar events in the future would help greatly advance the fundamental research efforts.

When discussing his views on policy-relevant research, David Goroff emphasized the importance of posing good questions, rather than focusing on outcomes. He also called for moving from descriptive to normative theories. One of the major research challenges is the development of multiscale models—covering the micro (individual) to macro (population) levels—and understanding the appropriateness of particular models for particular scales. STI modelling experts should aim to learn from other sciences that use systems-science approaches.

Applied Research

STI models are also developed within different government institutions and agencies and often lack wider exposure. The “Case studies” presentations were especially helpful in providing insights into the possibilities and challenges of carrying out applied research using modeling. Guru Madhavan, for example, emphasized the importance of systems analysis approaches. He reiterated the importance of taking into account cultural factors. He also emphasized the importance of building tools, such as the one developed by his group for the measurement of the importance of vaccines, SMART Vaccines, which

are used by decision makers rather than model builders. There was a general agreement that there is often poor communication between model builders and users/stakeholders, at all stages from the initial design (what question is being asked, what assumptions are being made, what measures and metrics to use, etc.) to the interpretation and application of results to the real-world problem. This is further exasperated by a less than open and transparent modeling process that does not create and maintain buy-in from the very beginning of a project.

Cyberinfrastructure

Cyberinfrastructure, e.g., data and model repositories but also computing and visualization infrastructures, are highly beneficial for advancing STI modeling efforts. Many sciences have setup billion-dollar international data infrastructure and distributed computing systems in close collaboration with government and industry partners. Examples are meteorology (e.g., weather forecasts and hurricane and tornado prediction), epidemiology (e.g., predicting the next pandemic and identifying best intervention strategies), climate research (e.g., predicting future scenarios and setting carbon prices), or financial engineering (e.g., stock trading and pricing predictions). No such infrastructure exists yet for the study and management of STI, yet 80 percent of project effort is commonly spent on data acquisition, cleaning, interlinkage, and preprocessing. Furthermore, modeling STI resources have been spent on individual project level, despite the experiences in natural sciences where building a general infrastructure of commonly used data available to all has led to major advances (e.g., climate studies, astronomy, etc.). Successful STI modeling requires validation, iterative improvement, and a community of users; all of which could be provided via appropriate infrastructure. However, building such an infrastructure will require active partnerships among academia, government, and industry. Sandy Pentland argued for the need to bring algorithms to data that are either too big for efficient sharing or have serious privacy and security issues.

Education

Education and training was discussed in a number of contexts. There were discussions regarding current “data literacy” and often expressed concern that it is rather low. Going forward, it will be important to introduce computational modeling and example models into formal and informal education. Participants also discussed the increased need for the active involvement of stakeholders into partnerships with modelers—to build simple models that can be understood more easily and validated to help stakeholders determine their usefulness. At the same time, many agreed that there is an urgent need for researchers and other model builders and users to enhance their communication and visualization skills.

Outreach

Modeling results need to be communicated to different stakeholders. Conference participants agreed that simple models and tools that are easy to understand and use and visualizations of model results that anyone can understand are key to the adoption and usage of models. Participants also emphasized the importance of storytelling and the art of communicating major results/recommendations in a clear and simple message. Kevin Finneran, National Academies of Sciences, Engineering, and Medicine,

especially emphasized the importance of communication with non-scientists and provided excellent examples of how such communication can be achieved.

ModSTI Insights and Opportunities

Key insights gained from the conference presentations and discussions as well as rather timely opportunities for advancing R&D on and the implementation of STI models are presented here.

Modeling needs and implementation, data infrastructure, code repositories and standards, visualization and communication, as well as funding are particularly important and promising and are detailed here.

Modeling Needs and Implementation

Modeling research and development strongly depend on a detailed understanding of the problem at hand and the range of actions a decision maker can take. If the wrong problem is modeled or if suggested actions are infeasible (e.g., doubling the U.S. R&D funding budget) then model utility will be low.

Several speakers noted that there is a major difference between statistical significance and business relevance. Nachum Shacham, PayPal pointed out model costs using an example of “false positives” (unidentified malicious users that cost PayPal money) versus “false negatives” (valued customers with blocked accounts that cost PayPal reputation and might lead to bad press). He pointed out that nobody should trust the result of any one model but should take note if five different models predict the same result.

Kaye G. Husbands Fealing, Georgia Tech argued for a “speed dating” as a means to connect stakeholders and scientists/analysts, to look at collective problems (not just one-offs), and to develop a feasible and sustainable bridge of communication. Ultimately, experts need to work across disciplinary and institutional (academia, industry, government) boundaries to exploit synergies and to arrive at modeling results that are greater than the sum of their parts. Model developers (e.g., in academia and industry) should aim to “room in” with model users (policy and other decision makers).

Ben Shneiderman, University of Maryland argued for the need to combine basic and applied (contract) work, see *The New ABCs of Research. Achieving Breakthrough Collaborations* (Shneiderman, 2016).

Martin Meltzer, Centers for Disease Control and Prevention pointed out the high value of usable, simple models that answer real questions.

There was a major discussion of black-box models such as IBM Watson technology presented by Richard Ikeda, NIH versus models that help people understand the system as presented by Petra Ahrweiler, EA of Technology and Innovation Assessment GmbH, Germany, William Rouse, Stevens Institute of Technology and others.

Computational models will need to be vetted by experts and earn the trust of the scientific policy making community before many start using them in practice. The key to building trust is transparency and the engagement of all stakeholders in the design and application of STI models.

Bill Valdez, The Consultants International Group pointed out that different policy offices have different ability to absorb/implement models and there is a considerable resistance to the adoption of new tools and approaches in general. He pointed out that the Federal Government is the largest, most complex organization in the world, yet it is poorly understood and continues to use outdated decision support tools and processes. Models could be extremely useful when making resource allocation decisions, the promotion of agency missions, or crisis management. Systems dynamic modeling is considered the way to go yet not much has changed over the last decade when these approaches were first suggested.

Data Infrastructure

A common theme across all the presentations was the importance of high-quality and-high coverage data for high quality modeling results. Currently, many teams are cleaning, interlinking, and processing the very same data, often in slightly different ways—foregoing the ability to replicate results across team sites. There was consensus that while having “big data” on science and technology dynamics is extremely important for answering certain questions, “more data” is not and should not be the answer to modeling questions. Going forward, data sharing and joint data curation efforts should be explored and the setup of data repositories seems desirable. James Onken talked about the ongoing effort within NIH for data integration via linked data. Richard B. Freeman emphasized the importance of using scraped information from websites such as Amazon and cell phone data in addition to traditional survey data and to get better measures of innovation in economic statistics. Also, while a large number of modelers are using unstructured data, Dame Wendy Hall and others have emphasized the importance of the creations of ontologies and structured data.

Given that many high-quality datasets are held by industry (e.g., Web of Science and Scopus publication data, LinkedIn expertise profile data, Twitter or Instagram data) it seems highly desirable to work closely with industry.

Code Repository and Standards

Equally important are efficient means to share STI model code. Some teams are using GitHub.com but STI models will be hard to find among millions of open source projects.

Many conference participants agreed the time is ripe to focus energy and resources on building cyberinfrastructure and research community that support systematic research and (tool) development efforts. Instead of creating a new repository, it seems beneficial to build on and extend (or interlink) existing model repositories. Model repositories are commonly created by academic researchers, government institutions, or publishers.

Academic repositories are typically associated with a tool, e.g.,

- Agent Modeling Platform (AMP) project provides “extensible frameworks and exemplary tools for representing, editing, generating, executing and visualizing agent-based models (ABMs) and any other domain requiring spatial, behavioral and functional features.” (<http://www.eclipse.org/amp>).

- GAMA is a “modeling and simulation development environment for building spatially explicit agent-based simulations.” (<https://github.com/gama-platform>)
- NetLogo is a “multi-agent programmable modeling environment. It is used by tens of thousands of students, teachers and researchers worldwide. It also powers HubNet participatory simulations.” (<http://ccl.northwestern.edu/netlogo>)
- MASON is a “fast discrete-event multi-agent simulation library core in Java, designed to be the foundation for large custom-purpose Java simulations, and also to provide more than enough functionality for many lightweight simulation needs. MASON contains both a model library and an optional suite of visualization tools in 2D and 3D.” (<http://cs.gmu.edu/~eclab/projects/mason>)
- The Repast Suite is a “family of advanced, free, and open source agent-based modeling and simulation platforms that have collectively been under continuous development for over 15 years.” (<http://repast.sourceforge.net>)

They might also be created for specific research projects:

- For example, the [SIMIAN](#) project is funded by the Economic and Social Research Council to promote and develop social simulation in the UK. SIMIAN uses the SKIN model (Ahrweiler, Pyka, & Gilbert, 2004). (<https://github.com/InnovationNetworks/skin>).

Modeling efforts are also supported by scholarly societies:

- OpenABM is a “node in the CoMSES Network, providing a growing collection of tutorials and FAQs on agent-based modeling.” (<https://www.openabm.org>)

Government institutions aim to support sharing of datasets or tools. NSF’s SciSIP program maintains a listing of “Datasets, Graphics & Tools” pertinent to the Science of Science Policy (SOSP) community at http://www.scienceofsciencepolicy.net/datasets_tools.

Interagency Modeling and Analysis Group (IMAG)¹ and the Multiscale Modeling Consortium aim to grow the field of multiscale modeling in biomedical, biological and behavioral systems, to promote model sharing and the development of reusable multiscale models, and disseminate the models and insights arrived from the models to the larger biomedical, biological, and behavioral research community, among others. The Predictive Model Index lists over 100 reusable, sharable models in support of reproducible science, see presentation by Grace Peng, NIH.

The Centers for Disease Control and Prevention (CDC) made the “H1N1 Flu (Swine Flu): Preparedness Tools for Professionals” software available at <http://www.cdc.gov/h1n1flu/tools>. The page was developed during the 2009-2010 H1N1 pandemic, it has not been updated, and is being archived for historic and reference purposes only.

Publishers aim to ensure replicability of work by asking authors to submit datasets and models. Examples are The *Journal of Artificial Societies and Social Simulation* (JASSS),

¹ <https://www.imagwiki.nibib.nih.gov>

<http://jasss.soc.surrey.ac.uk/JASSS.html>), an interdisciplinary journal for the exploration and understanding of social processes by means of computer simulation; published since 1998, JASSS recommends authors to upload model code and associated documentation to the [CoMSES Net Computational Model Library](#). In June 2016, the CoMSES library features 352 agent-based models.

Industry has long embraced big data and advanced data mining, modelling, and visualization algorithms. Computational models are widely used in online recommendation services (e.g., those provided by Amazon or Netflix), by financial and insurance companies (e.g., to detect credit card fraud, estimate fees). Many companies use models internally to support strategic decision making and to guide investment decisions. While code is typically proprietary, close industry-academia-government collaborations are likely beneficial for all parties involved.

Visualization and Communication of Modeling Results

Global operation rooms that provide visualizations of current data and predictions of possible futures are commonplace in meteorology, finance, epidemiology, or defense and might soon be commonplace in support of funding, strategic intelligence, or policy decision making.

William Rouse, Stevens Institute of Technology showcased “policy flight simulators” that let decision makers fly the future before they write the check. His team uses a combination of commercial off-the-shelf tools (e.g., AnyLogic, D-3, Excel, R, Simio, Tableau, and Vensim) rather than writing software from scratch. This practice can enable creating a prototype interactive environment within a week or two, which in turn allows rapid user feedback and easy mid-course corrections.

Ben Shneiderman, University of Maryland demonstrated EventFlow, a novel tool for event sequence analytics that includes a timeline display showing all individual records and their point and interval events as well as an aggregated view of all the sequences in the dataset (<http://hcil.umd.edu/eventflow>) and NodeXL (<http://nodexl.codeplex.com>). He strongly argued for the need to understand data quality before any type of data analysis is conducted or visualizations are rendered. Blind usage of data is dangerous.

Kevin Finneran, National Academies of Sciences, Engineering, and Medicine argued for the importance of storytelling, i.e., merging data with narrative, when communicating (the value of) research results. He noted that “Stories are the primary way to connect to policy-makers.” and “Data can be used to support the stories.”

Katy Börner, Indiana University and her team are developing and prototyping “science forecasts,” a news show that communicates local and global developments in science, technology, and innovation to a general audience. In Spring 2015, a pilot episode was recorded featuring a moderator that explains trends using an animated map of science (analogous to a weather forecast) and a zoom into a specific research result on ‘using Twitter for detecting episodes of depression’ presented by Johan Bollen who is interviewed by Fred Cate, both faculty at Indiana University. A still image of the news can be seen in Figure 2.

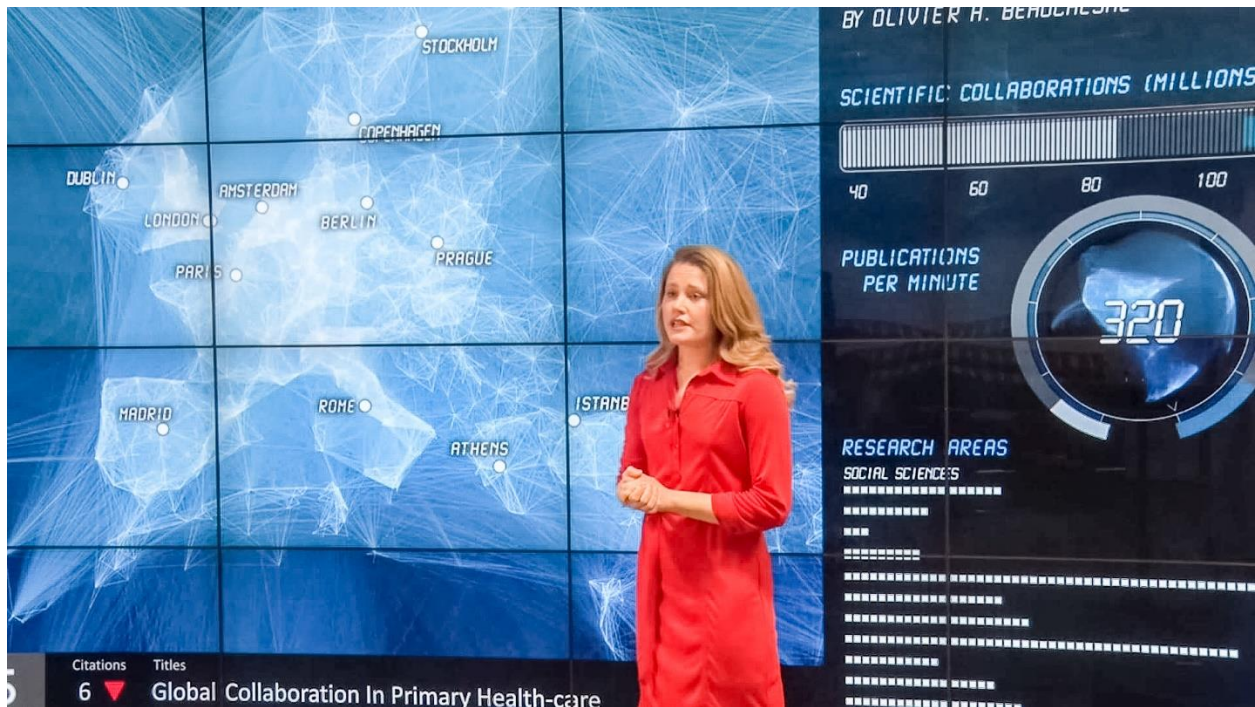


Figure 2: "Science Forecast," recorded at IU, presents interviews and animated maps of scientific activity in a manner similar to weather forecasts. The program demonstrates the power of data and visual analytics to provide up-to-date news on science trends and developments.

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However, the implementation and validation of computational models is costly. A key insight from the conference is the fact that just like it is common to set aside 10% of the overall budget for program evaluation, it seems appropriate to set a certain percentage of overall costs aside for computational modelling efforts. The concrete percentage amount will depend on an institutions interest (or mandate) to take all knowledge about a system, e.g., the science system, into account and to make decisions that lead to desirable futures.

ModSTI Outlook

In 2007, *Issues in Science and Technology* published "The Promise of Data-Driven Policymaking" by Daniel Esty & Reece Rushing. In 2016, the same magazine published "Data-Driven Science Policy"

² http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=501084

(Börner, 2016). The articles point out that in the corporate sector, a wide variety of data-driven approaches are used to boost profits, including systems to improve performance and reliability, evaluate the success of advertising campaigns, and determine optimal pricing. They argue for the need and discuss the premise of data-driven decision making in STI (including policy making)—using large-scale, high-quality datasets and computational means to inform human decision makers.

During the two-day conference, participants presented and discussed a wide range of mathematical, statistical, and computational models that were developed and implemented in a variety of settings. While the emphasis was on the power of models to advance future decisions, the presentations and discussions emphasized the usefulness of models to simulate, explain, and communicate the past, present, and future.

One two-day event will not suffice to bridge the gap between academic research ambitions, industry capabilities, and model needs by policy makers. A more continuous, long-term discussion and close collaboration is required to arrive at truly useful models that are widely adopted by science policy makers. A conference working group listserv was setup to accommodate interests of conference participants to share info on data, models, publications, events and continue the conversations in this research area. You are invited to join the discussion by signing up for and contributing via the modstl@iulist.indiana.edu list server.

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