



e_Connections

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Visual Analytics: a Grand Challenge in Science

On February 18, Jim Thomas, Director of the National Visualization and Analytics Center, gave a seminar entitled “Visual Analytics: a Grand Challenge in Science – Turning Information Overload into the Opportunity of the Decade” at the Virginia Bioinformatics Institute Conference Center. Thomas shared his vision of how visual analytics can help to

“detect the expected and discover the unexpected.” He emphasized how an interdisciplinary approach is essential to gain insight from the exponentially growing information and data that are coming at us from all directions.

Thomas earned a bachelor’s in mathematics from Eastern Washington University and a master’s degree in computer science from Washington State University. He is currently a Laboratory Fellow for the National

Security Directorate at Battelle’s Pacific Northwest National Laboratory, which he joined in 1976. He also directs the National Visualization and Analytics Center, which was founded by the Department of Homeland Security. Thomas acknowledged that around 10 years ago there was little interest in the visual analytics field as we know it today. However, 9/11 and the establishment of a visual analytics agenda from a forward-thinking group of researchers changed all that.

Thomas likens visual analytics to the last 12 inches between masses of information and the human mind where decisions are made. He describes the discipline as a contact sport, which not only requires a broad scientific agenda but also the close-knit interaction between researchers with know-how in cognitive and perceptual sciences, databases, knowledge structures, communications and decision sciences. According to Thomas, this emerging field of study requires talent from multiple disciplines including statistics, mathematics, information and computer sciences, knowledge and library sciences and many others working under the umbrella of team science.

Thomas remarked: “Throughout my career I have worked on different types of problems in varied disciplinary areas. I was working on the application of visualization to biological

data when I got attracted to the more ‘fuzzy’ area of text mining. The statistically driven tools we were able to develop for text mining turned out to be applicable to biology. There are synergies all around and that’s why it needs to be interdisciplinary to be successful.”

Thomas added: “Today an analyst needs to be able to look at around 3000 articles in about four hours to make meaningful decisions. A Boolean search is not sufficient to meet these needs, which will readily double or triple in a few more years. Data are not static. When you see an absence of information that can also be very revealing.” He added: “We really need to enable individuals in the field, like firemen, police officers and other emergency workers, with hand-held devices that are a significant evolution of the ones we have today. Mobile visualization analytics is at a very early stage but we will be making rapid in-roads into the development of scaleable reasoning systems.” He concluded: “It’s an exciting time to be working in visual analytics. I am sure we will see future breakthroughs and technologies that will help people derive insight from massive, dynamic and often conflicting data.”



Jim Thomas

In recognition of his contribution to science, the American Association of the Advancement of Science recently elected Thomas as a fellow for his “distinguished scientific and professional leadership in the field of visualization, including the recent foundation of the field of visual analysis.”

The National Visualization and Analytics Center (NVAC™) is a national and international resource providing strategic leadership and coordination for visual analytics technology and tools. NVAC supports the Department of Homeland Security’s mission to secure the homeland and protect the American people by giving analysts and emergency responders technology and capabilities to:

- Detect, prevent, and reduce the threat of terrorist attacks
- Identify and assess threats and vulnerabilities to our homeland
- Recover and minimize damage from terrorist attacks, should they occur

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CCF improves performance and capacity with Pillar storage platform



A recent addition to VBI's Core Computational Facility (CCF) is improving computational performance and capacity while reducing storage costs for the Institute and its customers. The Axiom 500 from Pillar Data Systems is an application-aware storage platform that combines two different storage environments into a single system that can be managed from one location. The system features both network-attached storage (NAS) and storage area network (SAN) functionalities. VBI's SAN infrastructure is primarily used to support the various research databases used at the Institute, featuring management systems such as Oracle, MySQL, and PostgreSQL. It also supports the large storage needs of specific groups at VBI, such as VBI's Core Laboratory Facility (CLF), which generates large amounts of data through its Roche GS-FLX™ genome sequencing system and other cutting-edge high-throughput technologies. The CCF's NAS services provide high-capacity access to personal and group file systems.

The Axiom 500 triples the Institute's storage capacity to 60 terabytes of data, which is roughly three times the amount of text-only information housed at the United States Library of Congress. While increasing the amount of computational storage space at VBI, the new system is actually more cost-effective, resulting in a decrease in service fees for CCF customers. The additional storage space also makes file duplication easier, strengthening the Institute's data back-up capabilities.

The Axiom 500 will house all of VBI's shared drives – network locations where employees can share large files and work groups can save and share important information – and provide more storage space for each faculty and staff member's home drive, where personal work data can be saved.

"The decision to add the Pillar Data System to our Core Computational Facility resources was an easy one," explained VBI's Chief Information Officer, Guy Cormier. "After looking at several systems, we found the Axiom 500 offers us more expansion capabilities and, most importantly, flexibility. The system doesn't require us to change our protocols. We can configure it to fit our needs."

VBI's CCF provides high-performance and high-throughput computing resources to support computational sciences, data mining, and access to a wide variety of biological applications. A cost-recovery service center, the CCF offers computational processing, database and system administration, data storage and archiving. The services are designed to assist researchers in the study of large-scale biological systems involving genes, proteins, and their interactions, as well as metabolic networks (systems biology).



VBI e_Connections

VBI e_Connections is a quarterly publication of the Virginia Bioinformatics Institute produced by the Public Relations team. The newsletter includes feature articles, technology updates as well as interviews that may be of interest to VBI's audiences. Contributions are welcomed.

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Bruno Sobral

Sobral Africa tour

VBI Executive and Scientific Director Bruno Sobral visited Kenya and Rwanda in November, 2007. The trip was the first aimed at seeking long-term, collaborative relationships with several sub-Saharan African countries that would allow first-hand research on pathogens while contributing to partner country goals and ultimately to world health goals. In Kenya, discussions were held with research teams at the International Livestock Research Institute (Nairobi) and the Kenya Medical Research Institute (Kisumu). In Rwanda, Sobral met with heads of state, including Professor Romain Murenzi, minister of technology, science, research and Information and Communication Technology (ICT); Mike Hughes, office of the president, strategic advisor on research, science, technology and ICT; Dr. Innocent Nyaruhirira, minister of state in charge of HIV/AIDS and other epidemics; and Professor Michael Kramer, director general, Center for Disease control.

Pereira named coordinator of international project

VBI Professor Andy Pereira is serving as coordinator of an international project for the Generation Challenge Programme (GCP), a broad network of partners from advanced research institutes and national programs collectively working to improve crop productivity in drought-prone environments. The goal of the project, "Validation of drought-response/resistance pathway genes by phenotypic analysis of mutants," is to identify rice genes involved in drought resistance. Pereira's partners for the project are the International Rice Research Institute (Philippines) and Huazhong Agricultural University (China). Pereira attended the annual GCP workshop in South Africa on September 12-15, 2007 to present his research group's role in the production of *HARDY*, a new type of rice that grows better and uses water more efficiently than other rice crops.



Chris Barrett

Barrett gives lecture at NSF-sponsored conference

VBI Professor and Director of the Network Dynamics and Simulation Science Laboratory Chris Barrett gave an invited presentation at *Frontiers in Transportation: Social Interactions*, a National Science Foundation-sponsored conference on information technology advances in transportation research, held in Amsterdam on October 12-18, 2007. In his presentation, "Interaction-Based Modeling of Population Dynamics and Infectious Disease", Barrett discussed high performance computing based approaches to population mobility, interdependent infrastructure and contagious diseases.

Tyler speaks at comparative genomics symposium

VBI Professor Brett Tyler was an invited speaker at the European Science Foundation-European Molecular Biology Organisation Symposium on "Comparative Genomics of Eukaryotic Microorganisms," which took place in Sant Feliu, Spain in late October, 2007. His presentation, "Oomycete pathogens: evolutionary origins and mechanisms of pathogenicity," described how comparisons among the genomes of several pathogens that successfully attack plants have provided insights into the mechanisms by which these microbes can defeat plant defenses.

Lawrence is invited presenter for Korean conference

VBI Assistant Professor Chris Lawrence gave an invited presentation, "*Alternaria* genomics: functional approaches for dissecting plant pathogenicity and fungal-associated airway disorders in humans," at the annual Korea Conference on Innovative Science and Technology in Jeju, South Korea on July 11-13, 2007. The conference, which featured the theme "Molecular Host-Parasite Interactions: New Horizon on Interface Biology," provides a forum for in-depth discussion on the current trends in molecular host parasite interactions.

VBI Scientific Publications

The landscape of human proteins interacting with viruses and other pathogens
Dyer MD, Murali TM, Sobral BW

PLoS Pathogens 2008 4(2): e32 doi:10.1371/journal.ppat.0040032

Researchers at the Virginia Bioinformatics Institute (VBI) and the Department of Computer Science at Virginia Tech have provided the first global analysis of human proteins interacting with viral proteins and proteins in other pathogens. The scientists examined publicly available experimental data for 190 different pathogens that comprise 10 477 interactions between human and pathogen proteins. This approach provides a highly detailed network map of human proteins interfacing with proteins in different pathogens. The network of interactions was published recently in the journal *PLoS Pathogens* and reveals possible key intervention points for the future development of therapeutics against infectious diseases.

Mathematicians uncover Sophie Germain's contribution to number theory



Sophie Germain was the first woman known for important original research in mathematics. A new investigation suggests that her stature as a number theorist is worthy of substantial elevation

"Germain had developed a sophisticated plan for proving Fermat's Last Theorem in its entirety and may have been preparing to submit her work to the French Academy's competition on Fermat's Last Theorem"

Sophie Germain, a 19th century French mathematician known for her research in the field of mathematical physics, is now being recognized for her significant accomplishments in number theory, thanks to the efforts of a VBI researcher and his colleague.

New Mexico State University Mathematics Professor David Pengelley and Virginia Bioinformatics Institute Professor Reinhard Laubenbacher scoured the archives of the Bibliothèque Nationale in Paris, France, and uncovered Germain's handwritten manuscripts and correspondence from around 1819 that include more mathematically sophisticated work in number theory than had originally been known. Laubenbacher and Pengelley presented their findings, which are featured in the paper "Voici ce que j'ai trouvé:¹ Sophie Germain's grand plan to prove Fermat's Last Theorem," at the Joint Mathematics Meeting in San Diego, Ca. on January 6-9. In the paper, the authors explore the greater scope of Germain's work to reveal its importance and argue that her recognition as a number theorist is in need of a major reevaluation.

Germain is widely known for her work on Fermat's Last Theorem, which states that if an integer n is greater than 2, then the equation $a^n + b^n = c^n$ has no solutions in non-zero whole numbers a , b , and c . "Sophie Germain's Theorem," which provides a partial insight into Fermat's Last Theorem, is respected by number

theorists but only garnered a mention in a footnote of a published paper by famed mathematician Adrien-Marie Legendre. Laubenbacher and Pengelley found that her work on the theorem was much more extensive than Legendre gave her credit for. Through their research, they found that Germain had developed a sophisticated plan for proving Fermat's Last Theorem in its entirety and may have been preparing to submit her work to the French Academy's competition on Fermat's Last Theorem.

Germain's mathematical approaches focused more on large, multifaceted theoretical techniques rather than attempts to solve certain components of the theorem, which was the method being used by others during this time period. For hundreds of years mathematicians have unsuccessfully attempted to prove the famous theorem, until 1994 when British mathematician Andrew Wiles discovered the solution.

Gender swap

Unable to receive a formal education in mathematics or acceptance into the academic community because of her gender, Germain's work was never published, packed away within 2,000 pages of work at the Bibliothèque Nationale. She shared her ongoing work on the theorem in a letter to German mathematician Carl Friedrich Gauss under a male pseudonym. Her inability to formally share her work with other mathematicians also forced Germain

to work in isolation, which made her susceptible to undetected mistakes. While Germain never actually proved Fermat's Last Theorem in its entirety, Laubenbacher and Pengelley found that her use of powerful theoretical techniques are comparable to the approaches used by mathematicians almost 100 years later and place her at the forefront of number theory research in the early nineteenth century.

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¹ "Here is what I have found:"