P.C. ROSSIN COLLEGE OF ENGINEERING AND APPLIED SCIENCE



Welcome to the 14th issue of Resolve, a magazine dedicated to research and educational innovation in the P.C. Rossin College of Engineering and Applied Science at Lehigh University.

Much has been written in recent years about the explosion of data being generated by the Internet and mobile devices and the manner in which this is changing the way we communicate and make decisions.

This phenomenon is often popularly referred to as Big Data, but the term Big Analytics more accurately captures the dual nature of the challenges and opportunities posed by the next phase of the Information Age. READ MORE >



—S. DAVID WU Dean & lacocca Professor

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T ARCHIVE

THE ERA OF BIG ANALYTICS

FINDING MEANING IN THE EXPANDING IMMENSITY OF DATA

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Making the most out of Big Analytics

Welcome to the 14th issue of Resolve, a magazine dedicated to research and educational innovation in the P.C. Rossin College of Engineering and Applied Science at Lehigh University.

Much has been written in recent years about the explosion of data being generated by the Internet and mobile devices and the manner in which this is changing the way we communicate and make decisions.

This phenomenon is often popularly referred to as Big Data, but the term Big Analytics more accurately captures the dual nature of the challenges and opportunities posed by the next phase of the Information Age.

At Lehigh, we define Big Analytics as the science surrounding the study of problems that involve massive amounts of data and/or large-scale computations. The promise of Big Analytics is twofold: It will enable us to extract greater meaning from huge sets of data, much of it contained

in ever-evolving and unstructured formats such as videos, emails, click streams and tweets. It will also make it possible to study climate shifts, nuclear fusion, radiation therapies and other phenomena that are too complex to reproduce and observe in a controlled environment.

In short, Big Analytics endeavors to transform data into insight and help us make more intelligent decisions. This requires new methods of searching, processing, storage and networking, along with upgraded information theory.

The scope of the problems to which Big Analytics can be applied is limited only by the imagination, ranging from healthcare to the electrical grid to the behavior of consumers and that of social media users. Lehigh's researchers in this area, as you'll see in our cover story on page 12, bring to the challenge a richness of expertise in data mining, search algorithms, optimization, information theory, machine learning and more. The problems they study span many disciplines, ranging from biological systems to the electrical grid and even including journalism and 19th-century American literature. Their goal is to add a fourth 'V'—veracity to the three V's of volume, velocity and



variety traditionally associated with Big Analytics. Several other articles in this issue of *Resolve* are related in one way or another to Big Analytics. The Q and A on page 8 features Robert Kahn, who played a critical role at the Advanced Research Projects Agency four decades ago in inventing the communication protocols

that support the Internet. A feature article on page 18 describes the efforts of Brian Chen, a bioinformatics expert, and his



to develop a noninvasive method of targeting cells with terahertz sensors.

On page 22, you can read about our new master's of engineering program in Technical Entrepreneurship, in which students work in teams to develop and test new products, study markets and launch businesses.

"Our goal at Lehigh is to add a fourth 'V'—veracity—to the three V's of volume, velocity and variety that are traditionally associated with Big Analytics." —S. David Wu

students to map and model the arrangements of atoms in protein molecules and thus help biologists better perceive the subtle differences and similarities between related molecules.

Another article with a life sciences angle appears on page 16. Xuanhong Cheng, a materials scientist, and James Hwang, an electrical engineer, have received a second round of funding from the U.S. Department of Defense I hope you enjoy this issue of *Resolve*. Please drop me a note to share your thoughts and comments.

Daville

S. David Wu, *Dean and Iacocca Professor* P.C. Rossin College of Engineering and Applied Science david.wu@lehigh.edu

Finding surface tension in compliant solid materials

Jagota's group also replicated Neumann's triangle, which describes the surface tensions of three immiscible liquids in equilibrium, replacing one liquid with a solid elastomer. A liquid has surface tension because, while its interior molecules are pushed and pulled in every direction by neighboring molecules, those at the surface have only half as many neighbors to interact with. The resulting density change of molecules near the surface causes a drop of water to form a sphere and enables a water strider to walk on water despite its greater density.

By contrast, says Anand Jagota, the surface tension of solid materials has seemed a moot point. Technically, it exists, but its



force is usually too weak to deform a solid by more than an angstrom.

Jagota, director of Lehigh's bioengineering program, has long wondered if some solids might exhibit surface tension. At the Leibniz Institute for New Materials (INM) in Germany and at Cornell University, he and his collaborators experimented with rubber-like elastomers and a more compliant gelatin similar in stiffness to human tissue. They patterned the elastomer with ripples measuring microns in depth, covered

> it with a gel and exposed it to air. Optical microscopy revealed that the gel faithfully replicated the surface topography of the elastomer.

When it was removed from the elastomer, however, the gel flattened almost instantaneously. It continued to match the peaks and valleys of the elastomer's ripples, but with significantly diminished features.

"We wondered if the gel would be an exact replica of the elastomer," says Jagota. "The gel had filled all the undulations in the elastomer, but as soon as we removed it, a pent-up force acted immediately to flatten it."

The group reported their results in *Physical Review E.* Jagota's coauthors were Animangsu Ghatak '03 Ph.D. of the Indian Institute of Technology at Kanpur, and Dadhichi Paretkar, formerly of INM and now a research associate at Lehigh. "Our results show that surface tension of soft solids drives significant deformation, and that the latter can be used to determine the former," they wrote.

The discovery, says Jagota, should motivate scientists to rethink many assumptions. "As a basic mechanical force, surface tension in compliant solids will play a role in all mechanical phenomena involving compliant materials, especially biomaterials. How do things fracture, stick, slide, have friction, deform? What are the elastic forces that resist a cell when it spreads on a gel? How strongly do dust particles stick to the inside of a lung?

"We're going to have to rethink many of the questions involving compliant materials." **0**

Open contours take cell's measure

Advanced imaging techniques make it possible to see the interior of the cell with greater clarity than ever. Now, a new software program is enabling researchers to go a step further and quantitatively analyze the thin filaments of actin protein that are critical to cell division and the formation of the cell's cytoskeleton.

Stretching Open Active Contours (SOACs) has been developed by a team led by Xiaolei Huang, associate professor of computer science and engineering, and Dimitrios Vavylonis, associate professor of physics in Lehigh's College of Arts and Sciences. Vavylonis and Huang have a five-year grant from NIH.

SOACs uses a quantitative image analysis algorithm known as "active contours" or "snakes" that detects filaments, locates their centerlines, delineates them from their networks and pinpoints filament junctions.

The software overcomes low signal-to-noise ratio, nonuniform intensity and width along filaments, faint filaments, intersecting and overlapping filaments, and the presence of non-filament structures. Multiple snakes can act in concert to extract a complete meshwork of actin filaments.

SOACs measures the rigidity of the filaments and the cables they form, their curvature and spatial distribution, and the changes these features undergo over time. It quantifies the brightness or dimness of the filament cables, which helps reveal the concentration of the filaments. Active contours are a common computer vision technique for delineating object outlines. Huang's students—Hongsheng Li, now associate professor at the University of Electronic Science and Technology in Chengdu, China, and Ph.D. candidate Ting Xu—helped develop the program that makes the contours open and stretch.

"Each contour," says Huang, "is like an intelligent curve or robot. They work together to locate and extract the centerline of a complex network. SOACs can be applied to all kinds of polymeric networks, including actin networks and microtubules;

they can also be useful in extracting capillaries and even neural networks."

Because of actin proteins' role in the division of all human cells, includ-



ing cancerous cells, the researchers hope that learning more about them will aid in the search for cancer therapies based on an advanced understanding of cellular function.





SOACs can extract networks of actin filaments in yeast cells and in other polymeric networks such as microtubules and capillaries.

Researchers advance the art of drug testing

Working at the nanoscale, scientists and engineers take aim at cancer cells.

On a rectangular chip slightly smaller than a person's finger, three researchers are writing what they hope will be the blueprint for the future of drug testing.

Yaling Liu, Linda Lowe-Krentz and Daniel Ou-Yang are etching the chip with channels that mimic the branching capillaries of the human lung and are coated with human endothelial, or blood vessel, cells.

Their goal is to determine how drugs

can be made to kill cancerous cells without harming healthy cells and tissue. They also want to reduce the cost of drug tests and the time it takes to run them.

Toward these ends, the researchers are studying cell behavior to learn more about how cells send signals to each other, how they are affected by blood flow, and how they can be studied outside the body.

The group, which recently received a three-year grant from the National Institutes of Health, includes three perspectives. Liu, an assistant professor of mechanical engineering and mechanics, studies interfacial phenomena at the micro- and nanoscale of biological systems. Lowe-Krentz, a professor of biological sciences in Lehigh's College of Arts and Sciences (CAS), studies the changes that cells undergo in response to blood flow. Ou-Yang, a professor of physics in the CAS, has developed novel methods of using microscopy and lasers, including "optical tweezers," to observe cell activities at the nanoscale.

By conducting tests on a chip, says Liu, researchers can approximate the environment a drug encounters inside the human body. Each chip costs less than a dollar to make. Multiple tests can be run simultaneously on a series of chips. Size is another advantage. In a test, the small chip uses only about a tenth of the amount of drug and tissue required by conventional testing methods.

"The chip enables us to grow human cells and observe a drug's effect on them



With an NIH grant, Lowe-Krentz, Liu and Ou-Yang are learning to grow human endothelial cells on channels patterned into a finger-sized chip.

in their natural environment," says Liu. "This will make it possible to do screenings much more quickly and shorten the research cycle."

Liu and his students fabricate rectangular chips from a polymeric material. Using

computer-aided design, they etch the chips with a pattern that resembles the lung's bifurcating geometry, with channels ranging in width from arteries (about 1 cm) to capillaries (10 microns).

The team will engineer the chip so it stretches like the breathing lung. A computer-controlled syringe will control the rate at which the drug is pumped into the chip coating. This flow rate affects cell health and cell signaling.

The design, elastic chip material and syringe, says Liu, enable the chip to

Bio-systems Dynamics Summer Institute, which is funded by the Howard Hughes Medical Institute.

When the chip is coated with endothelial cells, the researchers will treat the cells with a chemical that inflames the cells similar to the way cancer does. They will then inject the device with a blood solution containing nanoparticles hitched with a drug, an antibody and a fluorescent marker.

The antibody will cause the nanoparticle to bind only to cells that express the kind of receptor that cancer cells express. When binding occurs, the particles will release the drugs they are carrying.

The fluorescent marker will enable the researchers, using scanning laser confocal microscopy, to track the nanoparticles and their interactions with cells.

"Confocal microscopy works almost like an MRI," says Ou-Yang. "We scan a plane and illuminate each point of interest and then advance to the next sheet and repeat the process. The computer regenerates these images into a 3-D composite."

"The chip enables us to grow human cells and observe a drug's effect on them in their natural environment." —Yaling Liu

achieve a credible imitation of human breathing and blood flow patterns.

The next challenge is to coax endothelial cells to adhere to, and grow on, the channels of the chip.

"Growing cells has been called both a science and an art," says Lowe-Krentz. "As blood vessels develop, a single cell moves out and is followed by other cells. If too many cells follow, they can clog the new branches; if not enough follow, the cells don't cover the surface of the channel."

Liu's and Lowe-Krentz's students tackled this task through Lehigh's

The imaging technique will enable the group to quantify the percentage of the nanoparticles that bind to the cancerlike cells and thus measure the particles' success in finding their targets. The team will also correlate binding effectiveness with size by coating particles of various sizes with different fluorescent markers.

In the future, the researchers plan to coat the chip with multiple layers of cells with a porous membrane. This will enable them to study how cancer cells metastasize and migrate across blood vessels.

NANOBRIEFS



Bacteria offer quantum aid in methanol production

Backed by a \$2 million grant from NSF's Division of Emerging Frontiers in Research and Innovation (EFRI), a research team is working to create a promising new method of producing renewable fuel.

Using only carbon dioxide, sunlight and water, the researchers hope to perfect a green, low-cost process that could enable the production of methanol which can be used as fuel for cars, heating appliances, electricity generation and more—at commercial scale.

The EFRI award builds on the success of two Lehigh grants that enabled chemical and bioengineering professors Steve McIntosh and Bryan Berger to produce low-cost quantum dots (QDs) from bacteria.

QDs, small semiconductor particles, have potential in transistors, solar cells, LEDs, lasers, medical imaging and even quantum computing. They are expensive to make, as they require the use of toxic solvents and chemicals at elevated temperatures. Berger's novel idea to produce QDs from bacteria makes this technology green and affordable.

McIntosh and Berger worked with Chris Kiely, professor of materials science and engineering, to develop a low-cost method of producing QDs in bacteria. The team also includes biological sciences professor Robert Skibbens of Lehigh's College of Arts and Sciences and Syracuse University chemist Ivan Korendovych.

The researchers will couple the QDs with a series of yeast-synthesized enzymes. The QDs will capture the energy in sunlight to generate an energetic electron and electron hole pair. These excited species catalyze the removal of hydrogen from water and carbon from CO₂, and produce methanol, a renewable liquid fuel, in a continuous flow process.

The group's unique biosynthetic process to produce QDs, says McIntosh, enables control of the dots' particle size and, with that, the wavelength and energy of light captured. It is cheaper than using precious metal catalysts, and it makes large-scale production of liquid fuels far more feasible.

"The biosynthetic QDs not only allow us to design processes to produce liquid fuel at dramatically reduced cost, but also enable the development of an environmentally friendly, bio-inspired process unlike current approaches that rely on high temperatures, pressures, toxic solvents and precious metal catalysts," Berger says.

"This unique approach to liquid fuel synthesis will reduce both cost and environmental impact."

"In the process of trying to achieve our goals on this project, we also will learn valuable lessons that will advance science in other ways," says McIntosh. "Making QDs more cheaply and efficiently has many applications, such as efficient lighting, biomedical imaging and displays.

"Currently, there is no commercial route to directly and photocatalytically produce liquid fuels. Certainly, using sunlight to create liquid fuel is a high-risk, high-reward proposition, but that is what is so exciting. The implications for our nation's economy are significant." •

Streamlining high-quality plastics

Everything from the casing on your cell phone to the panels on your car is made of plastic that is manufactured using injection molding, by far the most common way of forming plastic products.

John Coulter, professor of mechanical engineering and mechanics, studies injection molding to help industries produce parts more efficiently. About 70 percent of the world's plastic products, he says, are made using cold runner injection molding. More intricate parts, including many plastics for medical applications, are produced using hot runner injection molding, which reduces the amount of costly plastic that is wasted.

The "runner" is the channel through which molten plastic travels into a mold. In cold runner injection molding, the runner solidifies, slowing production, and must be recycled or discarded. Hot runner injection molding produces parts more rapidly, and the runner never solidifies.

"You can save money by eliminating runner scrap," says Coulter, "and you can make more money by manufacturing parts more rapidly.

"Hot runner systems use more energy and pose maintenance challenges, but they can be cost-efficient with high-volume production of expensive, high-performance plastics."

Coulter's research focuses on computer, medical, optical and electronics products that use high-performance plastics. Because they are expensive polymers, companies want to use hot runner molding, but engineers must first solve the molecular degradation and other challenges posed by hot runner injection molding.

Coulter and his team study these materials as a function of time and position throughout the process. "For example, if a plastic stays hot too long, we look for the degraded spots, usually in the runner," he says. "Through computer modeling, we reconfigure things until we obtain the desired results."

The work is funded by the Research for Advanced Manufacturing in Pennsylvania, a partnership of Lehigh and Carnegie-Mellon Universities funded through the Pennsylvania Department of Community and Economic Development.

Coulter is collaborating with TE Connectivity, a leader in the connector products industry. The goal is to improve TE's high-precision manufacturing process by switching from cold runner injection molding to a hybrid system that combines cold and hot runner processes.

Extrusion for greener aluminum recycling

Solid state method cuts energy use while yielding improved mechanical properties.

Aluminum recycling has become a successful business since its inception a century ago. Nearly a third of the aluminum produced in the United States is made from aluminum scraps that have been recycled in a process—usually remelting—that uses only 5 to 10 percent

of the energy it takes to extract aluminum from mined bauxite ore.

But there are limitations to the remelting of aluminum, says Wojciech Misiolek, the director of Lehigh's Institute for Metal Forming and the Loewy Chair in Materials Forming and Processing.

Significant metal losses can occur when aluminum is remelted. Machine chips and other fine pieces of scrap are difficult to remelt. Contamination and impurities can cause the mechanical properties of recycled aluminum, especially its strength and ductility, to be inferior to those of pure aluminum. And remelting itself is energy-intensive.

In an effort to make aluminum production more sustainable, materials scientists are investigating solid state recycling of aluminum chips by extrusion, which promises higher metal yield, and lower heat use and energy consumption, than conventional recycling based on remelting.

A group that includes researchers from Lehigh and the Technical University (TU) of Dortmund in Germany has found that using special extrusion dies improves the mechanical properties of recycled aluminum by allowing more strain and shearing during metal flow.

Using transmission electron microscopy (TEM), the group is comparing the evolution of the microstructure, including the size and distribution of critical grain boundaries, of aluminum that is extruded through three different types of dies.

In the past year, the group has reported its results twice in *Materials Science and Engineering A* and once in the CIRP Annals of Manufacturing Technology.

In its experiments, the group processed machined aluminum chips into a cylindrically shaped billet and extruded the billet, pushing it through a die.

As aluminum flows through a die, it changes in shape and size.

Shearing occurs as the rate of flow increases and decreases, causing the fracture of an oxide layer, which covers each chip and can act as a barrier that prevents bonding.

The researchers' goal is to learn the amounts of shearing and deformation that promote

optimal bonding between the aluminum chips. They hope to do this by guiding the development of the aluminum's microstructure through the controlled fracture and dispersion of the oxide.

"We are trying to understand the critical conditions necessary to guarantee the good bonding of chips," says Misiolek. "Our goal is to control the microstructure and improve the mechanical properties of the aluminum."

While a continuous oxide layer can impede material bonding, says Misiolek, the researchers have learned that the right amount of the fractured oxide particles can result in a new and promising microstructure.

"TEM allows us to determine what shearing conditions are necessary to break the oxide layer and simultaneously preserve it to such an extent that it acts as a barrier to the growth of grain boundaries.

"We want to find this 'sweet spot' in shearing. We're hoping this will enable us to control the mechanical properties of aluminum, especially its strength and ductility."

The TU Dortmund researchers experimented with a conventional flat-face die used in the production of solid aluminum profiles, a porthole die used mostly to make complex hollow and semi-hollow profiles, and an ECAP (Equal Channel Angular Pressing) die, which guarantees the highest level of shear deformation and, therefore, modification of the microstructure.

While the aluminum extruded through the porthole dies possessed 80 percent more ductility than the aluminum extruded through the flat-face die, the researchers said, "the use of the ECAP die led to the highest strength and ductility of chipbased extrudates for the three dies."

Masashi Watanabe, associate professor of materials science and engineering at Lehigh, obtained TEM images of the microstructure of the recycled aluminum.

"With TEM, we can see grains, dislocations and other defects in the microstructure," said Watanabe. "We were able to confirm that even at a lower temperature, severe plastic deformation [caused by the extrusion] changed the microstructure significantly, creating nanosized grains that improved the mechanical properties."

In 2011-12, Misiolek spent six months at TU Dortmund's Institute for Metal Forming and Light Construction as Mercator Visiting Professor. His stay was funded by the German Research Foundation. Last year, Matthias Haase of TU Dortmund spent two months as a visiting researcher at Lehigh.

Other collaborators are Ph.D. candidates Volkan Güley and Ahmet Güzel, and Dr. Andreas Jäger, Dr. Nooman Ben Khalifa, Prof. Matthias Kleiner and Prof. A. Erman Tekkaya, all of TU Dortmund; and Lehigh Ph.D. candidate Joseph C. Sabol. **O** With TEM, Watanabe (below) observes grains, dislocations and other defects in the aluminum microstructure. A micrograph (center) shows grain growth prevented by a chip boundary in a chipbased specimen.

A. CHIP BOUNDARY B. COARSE GRAIN C. FINE GRAIN





UHD's promise: "The future has just begun"

A new semiconducting material proves its mettle with increased size and current demands.

New format, high definition displays on the way to consumers will bring a level of verisimilitude to home television screens that beggars belief.



Graduate student Forough Mahmoudabadi is helping Hatalis improve the performance of IGZO transistors.

"The images on these new screens are just astonishingly beautiful," says Miltos Hatalis, professor of electrical and computer engineering. "You can get very close to the screen, and the image is like nature."

Current HD displays have about 2 million pixels, arrayed in 2,000 columns by 1,000 rows. A new display format, called Ultra High Definition (UHD), is coming out in two varieties: 4k UHD with 4,000 columns and 2,000 rows of pixels, or 8 million pixels, and 8k UHD, which boasts 16 million pixels. The 4k UHD versions are just beginning to hit the market, albeit at princely prices and shy of performance levels designers seek to deliver.

Hatalis, who is working on innovations to make UHD a reality, says the increased performance requirements of the new format present much more than a fourfold challenge.

"UHD almost eliminates pixelation due to its higher resolution, but the amount of time given to address each row of pixels is proportionally reduced." This timeframe is compacted further by the quicker refresh rates the new screens need to render fast-moving 3-D images as vividly as life. With less time, the transistors and other components that activate each pixel must work faster and handle more current. However, given the higher resolution, the pixels must be smaller.

Bigger screens also require the display lines carrying the current to be longer, allowing increased parasitic resistance to sap signal strength.

These factors have outstripped the capacity of current HD display technologies, not to mention the inexorable demands of the future. The 8k UHD format—quadrupling the 4k UHD resolution and approaching that of IMAX—is already more than a concept.

To overcome these challenges, Hatalis is working with a new material indium gallium zinc oxide, or IGZO that can produce the smaller thin film transistor (TFT) components demanded by UHD formats while providing more than 10 times the current of TFTs now made with amorphous silicon.

Working in Lehigh's Display Research Laboratory, a unique facility that can produce prototype displays almost from scratch,

Hatalis has improved the manufacturing process to increase the performance and reliability of IGZO transistors. The delicate procedure involves several deposition steps, photolithography, etching and other techniques.

"We have found some treatments that make the transistors very robust," he says. "You have to go through a lot of steps putting down the material, heating it, etc. If you don't get each step of the process just right, you fail."

Besides display components that

create images, screens require drivers that process incoming signals and control pixels. Driver circuits are typically embedded into display panels, along the edges. Thin film transistors (TFTs)—common to all display technology and vital components of the drivers—ideally call for both N- and P-channel transistors. These transistors are complementary in that a charge that opens one will close the other, and vice versa—a useful quality in circuit design. IGZO lends itself only to N-channel transistors—at least for now.

"Working with Kamil Klier [University Distinguished Professor of Chemistry], we are exploring different materials to make the P-channel transistors, using elements in the IGZO family and amorphous metal oxides," says Hatalis. "We recently achieved interesting results doing computer simulations at Brookhaven National Lab."

In addition to the bigger format, new displays are being developed that will do away with the LED backlighting required by current LCD technology. Instead, AMOLED (active matrix organic LED) displays use diodes that produce light, rather than just modulate it, as do LCD diodes. AMOLED screens are used in smartphones and other small devices with pristine displays, but their production is expensive and not yet

> feasible for large TVs and monitors employing UHD for the consumer market.

Hatalis has received significant industry funding for his work with displays, and from the FlexTech Alliance for his flexible screen research.

He was among the first to publish in the field of flexible displays, and is experimenting with techniques that could put displays on car dashboards, clothing or even paper.

"The applications of flexible screens," he says, "are countless. The future has just begun." **G**



A dynamic fix for large-scale uncertainty

Scalable algorithms underlie continuous nonlinear optimization techniques.

Engineers optimizing the performance of a manufacturing plant seek to produce the greatest number of products at the least expense while meeting quality and safety standards.

The operators of an electrical power plant, by contrast, deal with variables and constraints that change rapidly and continuously, including the availability and cost of fuel sources and constantly fluctuating customer demand.

Software programs based on classical algorithms are well-suited to solve the first problem, says Frank Curtis, but their effectiveness is limited with the kind of dynamic optimization challenge posed by power plants.

Curtis, an assistant professor of industrial and systems engineering, recently received a fiveyear Early Career Research Program Award from the U.S. Department of Energy to develop dynamic, scalable algorithms for large-scale constrained optimization problems.

The grant will enable Curtis and his students to develop algorithms, or step-by-step mathematical methods, and work with researchers at DOE's Argonne National Laboratory to implement them in software that monitors and controls processes in complex systems.

The algorithms will also be used in software that solves design problems for systems that work in uncertainty.

"Our goal," says Curtis, "is to solve problems that require the use of continuous nonlinear optimization techniques. These problems include the design and construction of a network that has to be able to make countless decisions in real time.

"Another application would be chemical plants that have to monitor many factors at many stages of various processes."

Classical algorithms have long been used to solve nonlinear optimization problems, says Curtis, but they are not designed for real-time decision-making.

"Classical algorithms were never intended to be flexible or fluid. Dynamic algorithms are far more practical for modern problems that need to be solved continuously and in sequence. Our goal is to keep the parameters in a complex process in balance like the cruise control on a car.



"The key features of these new algorithms are that they will be fast, dynamic, and scalable to meet the computational requirements of scientists and researchers working to optimize large-scale, complex systems."

The DOE award is the second major grant Curtis has received in the last three years. In 2010, he received a three-year single-investigator grant from the National Science Foundation to develop nonlinear optimization algorithms for large-scale and nonsmooth applications.

Curtis, who has five Ph.D. students, collaborates with researchers at Johns Hopkins University, the University of Washington and Northwestern University. Curtis and his students work with DOE researchers to implement their algorithms in software that monitors processes in complex systems.

An intellectual infrastructure for structural engineers

Dan Frangopol, the Fazlur Rahman Khan Endowed Chair of Structural Engineering and Architecture, studies the life-cycle performance of structural systems. The American Society of Civil Engineers (ASCE) says his contributions over four decades "have not only saved time and money, but very likely also saved lives."

Frangopol's contributions include networks that unite the world's brightest structural engineers to solve the field's most vexing issues.

"New concepts profoundly reshape our thinking," Frangopol says. "We began moving in the direction of 'sustainability' before the term entered the popular lexicon. Professional networks integrate expertise and form the basis of wider-scale understanding."

In 1999 Frangopol helped found the International Association for Bridge Maintenance and Safety, which encompasses all aspects of bridge management—from repair, rehabilitation and safety to risk and economic implications. Frangopol also played a role in forming the International Association for Life-Cycle Civil Engineering and ASCE's Technical Council on Life-Cycle Performance, Safety, Reliability and Risk of Structural Systems.

Life-cycle engineering, a concept that Frangopol and his students helped pioneer, accounts for all variables that affect a structure's performance over time.

"In the most simplistic approach, decision making about the design of a structure is based solely on initial cost," says Frangopol. "Yet over time, the total cost of keeping the structure maintained and safe may be much larger than the initial cost. In emerging economies throughout the world, this has posed a problem. If minimum initial cost is the sole consideration, what happens when these structures start to deteriorate, all at once and in a relatively short timeframe?

"Design, maintenance and repair costs should be considered together, using life-cycle engineering. Decisions should be based on 'multi-criteria optimization under uncertainty' so we can balance conflicting objectives such as structural performance and cost."

Life-cycle engineering, says Frangopol, is linked inextricably to sustainability. "Besides a structure's physical properties and the intensity of the activity it supports, economic, political and social issues also impact its long-term viability. Our goal is to integrate these into a cohesive picture and allow for the best possible decisions to be made at the outset—long before unsatisfactory conditions occur."

Frangopol and his students work in Lehigh's Computational Laboratory for Life-Cycle Structural Engineering, where they optimize, predict and assess the performance of structural systems over service life. ()

STILL INVENTING THE FUTURE

INTERNET PIONEER SEEKS LASTING ACCESS TO INFORMATION.

Robert Kahn played a key role at ARPA (the Advanced Research Projects Agency) in helping invent the communication protocols that make possible the Internet. He is President and CEO of Corporation for National Research Initiatives (CNRI), which he founded in 1986 to foster research and development of the national information infrastructure. CNRI has developed an advanced architecture for information management (the Digital Object Architecture) and established the MEMS Exchange, which supports a national community of designers of micromechanical and nanotechnology devices and systems. Kahn received the Presidential Medal of Freedom in 2005. This year, he and four others were awarded the first Queen Elizabeth Prize for Engineering for "groundbreaking work that led to the Internet ... and initiated a communications revolution which has changed the world."

Q: Talk about the team of scientists you worked with to invent the protocols that led to the Internet.

A: The Internet is about the protocols and procedures that allow different components—networks and computers—to be connected and to work together as part of a global information system. A lot of work was done on networking and computer technology long before the Internet came around.

I had worked on ARPANET (sponsored by ARPA, later renamed DARPA, Defense Advanced Research Projects Agency), which was the world's first computer network and which used a novel switching technique called "packet switching". By the early 1970s, DARPA had sponsored the development of a number of different networks, and the question was how to interconnect them and the computers connected to them.

I wanted to better understand how computers

could communicate, especially if some networks to which they were connected were unreliable. At the time, I didn't fully understand the operating system side of the world, so I invited Vint Cerf, with whom I had worked with on testing the ARPANET, to collaborate with me on the Internet aspects. Together, we made the architecture stronger and better. A lot of people worked on other aspects; Vint and I developed the Transmission Control and Internet Protocols (TCP/IP) that are still used today. They are now the glue that holds the Internet together. **Q:** *Did you ever expect the Internet to become a place where people shop, gather socially, and*

search for news and entertainment?

A: I could imagine that, but it wasn't the purpose of our work at the time. Rather, it was to enable interconnection of networks and computers for the purpose of sharing resources such as programs,



storage and processing. DARPA's motivation for supporting this effort was computer network resource sharing. Computers were then quite expensive. Sharing resources among research groups would be more cost effective than providing each group with its own dedicated resource. Today, I'm concerned with how information is created and managed in the Internet such that users have reliable access to it and, potentially, that it provides dependable intergenerational access for years to come. This is basically a question of the interoperability of different information systems and their ability to share information, and for information access to persist over technological change well into the future. **Q**: Is the Internet fulfilling its potential for granting greater numbers of people access to information?

A: Perhaps a third of the world's people have Internet access of some kind today. The questions are: Will information be accessible in the Internet, can people afford it, what kind of information do they need, can they assimilate it, will there be open access? The biggest challenge is in some developing countries. Most individuals there have access to cell phone technology, but not necessarily to the Internet. There's a lot more work to do to get more people online.

Q: How has the Digital Object Architecture that you invented made it possible to manage information better?

A: Instead of moving undifferentiated information from one place to another, DOArchitecture enables the movement of structured information in the form of a digital object with an associated *unique persistent identifier*. If you access material on the digital bookshelf 100 years in the future, and if the information has been managed during that period of time to ensure its continued availability, you can find it using its identifier, even if the technology is radically different. That's one piece of it, persistence of identification for indefinite access.

The second piece is the ability to store and access these digital objects with repository technology that uses state-of-the-art storage technology. If the repository interface is based on identifiers, it is sufficient to access the information, provided, of course, you are authorized to access it. You need *interoperability* for information to flow seamlessly. Finally, *security* is important for everybody. Every resource in the Internet has an identity that can be used to validate resources and access digital information.

Q: How can CNRI's Handle System technology improve something like the online storage of medical records?

A: The Handle System technology is a component of DOArchitecture that resolves identifiers. It provides state information about digital objects, such as IP addresses, authentication information and public keys. For example, to retrieve your medical records, you would first provide the identifier of the digital object that contains your records. You would confirm that you're talking to the right place, and then ask for the information you want by providing its identifier; and they would likely ask you to verify who you are. This can all be done using identifiers. Overall, this approach can have a positive impact on online access to medical records.

Q: Has the explosive growth of the Internet surprised you?

A: Not really. A lot of what can be done on the Web today could have been done on the ARPANET in the early 1970s, such as email or file transfers. You have to differentiate between a surprising innovation that had no previous counterpart and a logical extrapolation of what previously was available although perhaps in a somewhat different form. While the widespread use of the Internet doesn't surprise me, what does surprise me is when something appears that you had no reason to anticipate. I don't mean to trivialize any of the recent Internet work. A lot of it is quite brilliant and is much better than what we did in the early days; however, much of it is also a logical extrapolation of what existed years ago.

Q: The Internet is one of the hallmark advances of the 20th century. Do you have a sense of pride in that achievement?

A: Yes, at some fundamental level, but I'm still pretty active in trying to evolve and extend Internet capabilities. Every now and then, though, there comes a visible reminder like the Queen Elizabeth Prize. When we started with the ARPANET we were treating it as a scientific problem. I suppose some people start out thinking they're going to change the world, but that's not what we set out to do.

I once was asked how we managed to get permission from all the governments of the world to build the Internet. The answer is: we didn't have to ask their permission because most people didn't think our work was going to amount to anything. So we had pretty much free running room.

Q: Is there an inevitable tradeoff between people's desire for greater access and speed and their desire for security?

A: The tradeoff is not between access speed and security, but between the private sector's desire for security and the more global needs of the public sector for law enforcement and national security. If those security issues could first be resolved, they could be dealt with technically at speed and with the right infrastructure support.

Q: Is it realistic for Internet users to expect privacy in an age when huge amounts of information are stored on public sites and accessible to government and private industry?

A: The real issues are what role government should play to protect citizens, and what expectations of privacy individual users should have. A lot of young kids today put their whole life story out on the Internet for everybody to see—what they did last night, what they're thinking about this morning. Maybe future generations will go the other route and say, "Gee, our parents wanted everything to hang out, but we don't think that's such a good idea." So I would say, stick around and let's see what actually happens. Ultimately, that's the best predictor of the future.



THE POWER OF A PULSE

A TEAM LOOKS PAST THE CELL MEMBRANE TO DNA SEQUENCING.

Xuanhong Cheng and James Hwang have developed a technique that enables live cells to be probed with focused beams in the terahertz range. Nature does not reveal its secrets to just anyone, and many of its mysteries are beyond our ability to perceive them with our unaided senses. Scientists have built massive tools like orbiting telescopes and supercolliders that can reveal hidden enigmas from the intergalactic scale down to the minuscule workings of subatomic particles.

If a team of Lehigh researchers is successful, one of the next high-tech tools to unveil the unseen will be a device that can identify substances at the molecular level—and potentially decipher DNA—and that will fit into the palm of your hand.

James Hwang, professor of electrical and computer



engineering; Xuanhong Cheng, assistant professor of materials science and engineering and bioengineering; and Cristiano Palego, a research scientist, are in the early stages of developing a handheld sensor that can identify bacteria quickly.

The immediate application is to detect pathogens in a combat zone or other securityrelated venue, and the team has received initial

and follow-up grants from the U.S. Defense Department. Assisting in the research are Caroline Multari and Yaqing Ning, Ph.D. candidates, and Caterina Merla, a visiting scientist from ENEA, an Italian government research agency.

The first phase of the project was to create a sensor to

determine if a given cell is alive or dead.

"It's a primary task," says Cheng, "because for a pathogen to be dangerous it generally has to be viable."

Testing for viability is typically done with optical instruments, which are bulky and do not lend themselves easily to miniaturization. Another method is to fire electrical pulses in a range of frequencies at a cell and see what bounces back, like radar. This technique, called a frequency domain electrical test, can be susceptible to false positives. Multiple dead cells, for example, can sometimes return a numerical value indicating a live cell.

To overcome this problem the team is using a time domain technique, firing a pulse at controlled intervals at target cells and analyzing the results.

"We're not experimenting with the frequency too much at the moment, as it has a thermal effect," says Palego. "The time-domain pulse excites the cell's components without heating up the cell."

"The beauty of time domain," says Hwang, the project's principal investigator, "is that you can easily generate a short pulse that encompasses many frequency components. But you have to disentangle the frequency domain data from the time-domain pulse; otherwise, it's a big mess. For that we need to do frequency domain studies."

The analysis of cell viability looks first to the cell membrane. If the membrane has been breached or has lost its integrity in some way, it's a good sign the cell is no longer viable. When excited by a pulse, the signature of the returning vibrations can show if a cell membrane has been compromised, much like the difference in tone between an intact drum head, which resounds emphatically when struck, and a split one, which returns a flaccid thud.

Working on mammalian cells, which are relatively large, the team has succeeded in this initial phase of the project. The next step is to obtain more information about the interior of the cell beyond the membrane. After the team targets smaller cells and organisms, eventually at the molecular level, it will seek to optimize and miniaturize its device.

Exciting molecules requires a focused beam in the terahertz range, says Cheng. "Larger wavelengths, even at the gigahertz level, will wash over molecules like a huge, rolling wave without creating any measurable activity in the molecule."

Terahertz waves, however, don't propagate well in fluid, or even humid air, and fluid is necessary to keep the target cells intact. The solution, says Hwang, hinges on positioning.

"We want to remove as much of the fluid between the sensor and the target as possible, keeping the cell alive, and getting the sensor right on the target," he says. "We're working on innovative technology to make that happen."

Making the tool workable as a handheld device increases the challenge. Calibration is an issue with sensors, so developing a technique that enables the device to quickly calibrate itself is crucial. Moreover, all the components must be scaled down, and data analysis, which is now done manually, must be automated.

"Eventually, we see all of this being miniaturized onto a single chip," says Palego. "CMOS [complementary metaloxide semiconductor] technology is very suitable for this kind of project and it is a common trend."

"One of the strengths of our team," says Cheng, "is the close relationship we have with collaborators who can do state-of-the-art CMOS production quickly and efficiently. Once we have the chip designed, we can go to large scale production rapidly."

The long-term goal of the project is to perform abbreviated DNA sequencing on target cells and to identify them unambiguously.

"This is the outer reaches of what we hope to do," says Cheng. The process would start by creating a small pore in the target cell with a tightly focused electric pulse. Cell contents could then be extracted from the cell interior through the pore. Because DNA has an electrical charge, a charged probe can coax it out.

"Graphene is an interesting material for this," says Palego, "and it could allow us to activate the pore, and use it as a tool." The pore itself could be used to obtain particular bits of information—such as the length of time it takes for a section of the unfurled DNA strand to pass through the pore—while doing an abbreviated sequencing of the DNA or highlighting a unique identifier.

"The technology is there, but there is plenty to do to get all the parameters right," says Cheng.

Military applications are the impetus for the project, says Palego, "but there are many other possibilities. On the medical side, these





include not just identifying cells but monitoring cells to check medication effectiveness, which could be done at home. Other potential applications include therapeutic uses, such as pulsing electromagnetic energy into cancer cells to disrupt their viability."

Cheng elaborated further: "The civil and medical possibilities are very broad. For example, instead of going to a lab for a blood analysis, you could have it done virtually anywhere with a tool like this. This would increase point-of-care possibilities for underserved populations."

Using CMOS technology, the researchers hope to develop a chip with sensors that can identify cells, confirm their viability and perform abbreviated DNA sequencing.



STORY BY RICHARD LALIBERTE

THE ERA OF BIG BIGHENTICS

LEHIGH RESEARCHERS ARE DEVELOPING TOOLS TO GRAPPLE WITH HUGE AMOUNTS OF DATA.

Consider what happens when you place an order with an Internet retail site such as Amazon.com. You search for a product and narrow preferences until the site finds an exact match from a sprawling inventory. The site analyzes a shipping system in which millions of items are in motion at once, calculates costs and estimates a delivery time. Money transfers from your bank to the vendor's, and information about your order goes to a warehouse, where computers find the item's physical location and track it as it's pulled, packaged and placed on precisely the right truck to bring your order to your exact address.

"Each step along the way is a huge data analysis problem," says Ted Ralphs, associate professor of industrial and systems engineering (ISE). "I

know how the systems work beneath the surface and the whole process still boggles my mind."

The use of information on a mindboggling scale is now commonplace

in the emerging world of what's become known as Big Data. Many people have become aware of the challenges, opportunities and, to some, threats of large-magnitude data analysis through debates about its role in national security and marketing. But Big Analyticsusing algorithms to sift through massive data sets in order to find patterns, reveal hidden correlations, make predictions and improve function in the most efficient way possible-also has the potential to dramatically enhance virtually every field of science, engineering, business and the humanities.

"Astronomical surveys of the heavens, weather measurements, gauges of loads on bridges, brain scans, genome mapping, social media they all generate massive amounts of data that are far beyond what any human could possibly take in," says Jeff Heflin, associate professor of computer science and engineering (CSE). "The question is, how can we make all this data useful?"

Harnessing the data explosion

In one sense, Big Data has been around a long time. Businesses, for example, have long grappled with the logistics of fulfilling orders and making deliveries. But several converging trends have enabled the tools for analyzing increasingly large and complex data sets to become more powerful than ever before. Lehigh researchers are using these new capabilities to tackle the challenges of Big Analytics on a number of levels, from boosting the precision of searches across vast amounts of information to evaluating the quality of results, predicting online behavior and making the most efficient use of computing power for faster and more valuable calculations.

Among the trends: "Computing and data storage are getting cheaper, and networking is getting better, so it's becoming cost-effective to capture and analyze lots of data in ways we couldn't imagine 10 years ago," says CSE associate professor Brian Davison.

At the same time, computing and hardware advances increasingly allow analytical tasks to be "Data might take the form of sound, images, video or information in Excel or Word—or website links, Facebook posts or online social connections." —Jeff Heflin

Brian Davison

distributed among multiple processing cores, machines or networks. "Big, interesting problems can't be calculated on a single machine," Davison says. "You need clusters of machines, which may be of different types." This approach, known as heterogeneous computing, divides large problems into smaller ones that different computers can solve concurrently, integrating their results.

Data itself is becoming more heterogeneous as well. In the past, digitized data was largely structured—meaning it followed well-defined database formats such as columns and rows that tended to be shared across platforms. Today, there's an explosion of unstructured data in widely different forms. "Data might take the form of sound, images, video or information in Excel or Word," Heflin says—or website links, Facebook posts or online social connections.

Even within a given format such as text, data elements can vastly differ. Variables range from file length to the meanings attached to specific words. (Does "fracking" refer to hydraulic fracturing or an expletive used in the futuristic world of *Battlestar Galactica*?)

"Putting data together for analysis creates challenges in matching schemas," or data structure, says Heflin. "Once you've made matches, you need to come up with ways to query efficiently across different databases so you're not wasting time and resources reviewing every possible source, including those that couldn't possibly have the answer."

Such challenges have led to advances in machine learning, in which advanced algorithms automate the discovery of patterns and trends so that computers can make predictions and come to accurate conclusions based on mathematical probabilities.

"One of the best examples of applying these analytical techniques on huge amounts of data is the development of the smart grid," Ralphs says. Already the focus of a research cluster at Lehigh called Integrated Networks for Electricity, the smart grid would overlay the nation's antiquated electrical system with a layer of information technology. By constantly monitoring itself and allowing real-time communication among utilities, users and other key elements of the electrical system, the smart grid would more easily integrate renewable but fluctuating sources of energy such as solar and wind. It would also offer consumers information about electrical demand and at-the-moment energy costs so they could buy electricity cheaper during off-peak hours—running the washing machine at night, for example, instead of during the hottest hours of a summer day.

> "The system will need to crunch huge amounts of data—sometimes within minutes—to make predictions about a vast number of variables," Ralphs says. These include what appliances people will be using at any given time, how much sun will shine and wind will

blow to generate electricity, which mainstay power sources such as nuclear reactors will need to be online, and what actions will be needed if demand and supply start to become unbalanced.

Searching for gold

Crunching large data sets to make correlations and predictions is already fueling big business. "The classic example is stores looking at purchases that tend to go together," Heflin says. Walmart, for example, mined its massive records of customer purchases and discovered that as hurricanes approach, people stock up not only on flashlights but Pop-Tarts. Placing the non-perishable pastry at the front of stores near other hurricane supplies boosted sales.

"The goal is to find patterns that aren't obvious," Heflin says. "When people open a wedding registry, it's easy to guess they're interested in honeymoon travel. More interesting and valuable would be to know that people from a specific ZIP code are most likely to take cruises. You can learn that from looking at massive amounts of data."

Heflin specializes in panning informational gold from the vast Internet data stream through the Semantic Web, an effort to promote common data formats that allow machines to process information more intelligently. One challenge is evaluating how much you can believe the information a search may turn up-"because it's well known that the Internet is 100 percent factual," Heflin savs with a wink.

Heflin evaluates information quality by looking for patterns such as inconsistencies across different sources of linked data. In 2012, a system that he and a team of students built won the Billion Triple Challenge, a highlevel competition at the International Semantic Web Conference in Boston.

"A triple is a digitized fact with a subject, predicate and object," Heflin says. "Our interface allowed us to browse about 30 billion triples in about 300,000 categories of data to reveal interesting phenomena, connections and errors."

For example, the system discovered that a popular online source of structured data had confused a British computer scientist with a jazz musician. "They had the same name, but different birthdates," Heflin says. "Triples about the scientist were using the same identifier as triples about the musician so they appeared online to be the same person." Such data sleuthing adds new tools that could help produce more fruitful search results.

Fruitful searching could also entail finding articles that not only are accurate but offer a particular perspective-

"A scientific basis for the

theories of data extraction

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-Eugene Perevalov

as revealed by algorithms that detect various forms of bias. Davison is developing such a model with funding from a Lehigh grant. "People have different worldviews when they write, particularly news," Davison says. "It might be a political or religious bias. a tendency to use big words, a fondness for sports analogies or a tone that's negative or sensational. Our goal is to recognize what the biases are so we can customize content to what a viewer really wants."

The algorithm would be able to score any article on a variety of perspectives and recommend similar articles-or alternatives. When researching any topic, you could easily use the system to seek a balanced view. That would offer an escape from what's been called "the filter bubble"-a phenomenon in

GEOMETRIC GOLD MINING

Trying to find meaning in Big Data, says Eugene Perevalov, can be like searching for gold.

"People get agitated about Big Data," says Perevalov, an associate professor of industrial and systems engineering. "They know there is useful information, but it's scarce, like tiny bits of gold in a huge amount of sand.

"Therefore, it's extremely important to develop a methodology for extracting value from junk."

Perevalov studies information theory and develops geometric models that quantify the data in large data sets, or "knowledge sources," the accuracy of this data and its relevance to questions posed by users.

Extraction, transmission and usage form the three links of the path, or journey, of any piece of useful information, he says, but while information transmission has been studied extensively by information theorists, extraction and usage have not yet received a comparable treatment.

A scientific basis for the theories of data extraction and usage, Perevalov says, would enable scientists to write scalable, efficient algorithms that enable users to make fuller use of raw data.

"We can quantify a knowledge source in an ad hoc way," he says,

"by asking it a series of questions and hoping to gradually stumble on the type of questions that it can answer well.

"But this is informal. I need an educated approach. To make a scientific description of a knowledge source, I make a geometric model first."

To obtain this model, Perevalov poses questions to large data sets and compares the answers he gets with the actual answers. This allows him to estimate the source's "knowledge structure," which, in general, takes the form of a tensor—a geometric object that has different magnitude in

every direction.

"Once we form the knowledge structure of a source, we can ask the source more educated questions. To solve the problem most effectively we have to strike an



optimal balance, with our questions, between the relevance of our question to the problem at

hand and the difficulty the source will have in answering that question. "There's a tradeoff curve between the accuracy and the relevance of information. You have to find this tradeoff for every problem by aligning the source to the problem."



Heflin (center) with Zachary Daniels '14 (second from right) and graduate students (l-r) Sambhawa Priya, Kelly Reynolds, Xingjan Zhang and Dizhao Song

"Our interface allowed us to browse about 30 billion triples in about 300,000 categories of data to reveal interesting phenomena, connections and errors." —Jeff Heflin



which your prior browsing history automatically personalizes and narrows the information a search reveals to you without you even realizing.

"Scoring biases could reinforce the filter bubble," Davison says. "But we give people a choice."

Parsing information with Big Analytics can help refine social media as well. In a paper titled "Predicting Popular Messages

in Twitter," Davison and graduate students Liangjie Hong and Ovidiu Dan analyzed more than 10 million tweets to determine why posts are retweeted.

"We found that Joe Random can do everything right and still not be retweeted," Davison says. "What determines retweeting are factors like whether you have a track record of posting worthwhile content, who follows you and whether the topic is already popular."

The paper won the Best Poster Award at the 2011 World Wide Web Conference in Hyderabad, India, and Hong is now a researcher at Yahoo! Labs.

In a follow-up project, Davison, Hong and graduate student Aziz S. Doumith tackled a more complicated question: Who will retweet what? "This model predicts individual interests and behavior based on what you've done in the past," Davison says. "We find this more interesting if the ultimate goal is to understand your interests and provide more of the information you really want."

Their paper—a finalist at the 2013 International Web Search and Data Mining Conference in Rome—suggests that such models could help sort through an overwhelming gush of social media information and pluck out messages you'll actually care about. Predicting retweets is also extremely valuable to companies.

"If someone has a million followers, it's obvious that people are paying attention," Davison says. "But if companies know that a person with a thousand followers today will have a half million next year, they can establish a relationship before that person becomes big."

The optimizing balance

Answering even relatively limited questions can consume enormous computing power if the scope of analysis is broad enough. "With current capabilities, it would take many lifetimes of the universe to create a computer that could make the perfect chess move every single time," says Heflin. However, the more limited goal of creating a program that can beat any human is more attainable.

"A large part of computer science is figuring out when it's time to back off and try for an algorithm that approximates what you're looking for, then figuring out when it's good enough to give you the quality you need," Heflin says.

Such optimization is a driving force behind analytics, and its methodologies often draw on game theory.

"When you have multiple decision makers —that is, players—each solving their own problems but affecting each other, you're in the game theory world," Ralphs says. One game theory model assumes groups of players are working against each other. "This is the kind of analysis the Defense Department uses in counterterrorism, and we've had a small grant from the Army to work on these kinds of problems."

A second model assumes players are cooperating. Delivery operations—like UPS bringing your order from Amazon. com—are a prime example. "They're a hierarchy of different subsystems ranging from a single truck driving around to fleets of trucks, warehouses, regional warehousing operations and on up," Ralphs says. Improvements in optimization, machine learning and data storage in recent years allow constant feedback between subsystems so that efficiencies are shared throughout the whole system almost as soon as they occur.

Ralphs develops software and chairs the Technical Leadership Council of a nonprofit, open-source research foundation called COIN-OR—short for Computational Infrastructure for Operations Research. "We develop tools that other people then use for specific applications," Ralphs says. "I'm passionate about these ground-level software methodologies because they have broad applications."

In medicine, for example, integrated analytics allow a treatment known as intensity-modulated radiation therapy to deliver optimal amounts of radiation to cancer tumors while avoiding healthy tissue. Making the system work entails using data from previous outcomes to predict effects, analyzing imagery to locate boundaries between healthy and cancerous tissue, and optimizing the function of the machine in real time as it delivers bursts of radiation in precisely calibrated doses to different areas of a patient's tumor.

"Big Analytics is an inherently multidisciplinary field because big problems need a lot of different perspectives to be properly understood," Heflin says. The amount of data, how fast it arrives, the form it takes and how accurate it is sometimes called the "four Vs" of volume, velocity, variety and veracity—"are each research areas in themselves," he adds.

This invites collaboration among researchers seeking the big picture. Heflin and Davison, for example, are exploring ways to combine their respective interests in structured and unstructured data. "If you only focus on one or the other, you're missing half the world," Davison says.

The tools that analyze data can also be applied to disciplines outside of science and engineering. Heflin has worked with Edward Whitley, English professor in Lehigh's College of Arts and Sciences and author of *The American Literature Scholar in the Digital Age*, to develop tools for analyzing a trove of digital data related to bohemians such as Walt Whitman who congregated in New York's lower Manhattan during the 19th century.

"It's a work in progress, but we hope to look at relationships and social structures that contributed to literary processes in this influential community," Heflin says.

"Some people want to develop analytic techniques while some people want to use them, and these people need to find each other," Ralphs says. "If it hasn't already, Big Analytics or Big Data will touch almost every aspect of life."

ROBOTS LEAVE THE NEST

Researcher develops agents that set and achieve goals while adjusting to changes in their environments.

The computing devices and software programs that enable the technology on which the modern world relies, says Hector Muñoz-Avila, can be likened to adolescents. Thanks to advanced algorithms, these systems, or agents, are now sufficiently intelligent to reason and to make responsible decisions—without adult supervision—in their own environments.

Muñoz-Avila, an associate professor of computer science and engineering, says algorithm-powered agents will soon be capable of investigating a complex problem, determining the most effective intermediate goals and taking action to achieve a long-range solution. In the process, agents will adjust to unexpected situations and learn from their environment, their cases and their mistakes.

They will achieve all of this without human control or guidance.

An agent—a robot or an automated computer game player—that is programmed with advanced algorithms can do many things not possible for a human being, says Muñoz-Avila. It can sift through thousands of stimuli and data points, pinpoint unusual patterns or anomalies, correct most of them in real-time and single out the complex abnormalities that require human intervention.

Muñoz-Avila, a pioneer in the new field of goal-driven autonomy (GDA), has a three-year grant from NSF to develop autonomous agents that dynamically identify and self-select their goals, and to test these agents in computer games.

"For a long time," he says, "scientists have told agents which goals to achieve. What we want to do now is to develop agents that autonomously select their own goals and accomplish them.

"A GDA agent follows a basic cycle. It has an expectation of something that will happen in an environment. When it detects an unexpected phenomenon, it attempts to explain the discrepancy between what it expected and what is actually happening. It is constantly checking when expectations are satisfied and when they are not, developing explanations for discrepancies and forming new goals to achieve them."

The applications of GDA agents include military planning, robotics, computer games and control systems for electrical grids and security networks.

Muñoz-Avila and his students have two goals—to improve and expand the knowledge that GDA agents acquire of their domains and to generalize the success of these agents to other domains and applications.

As autonomous computing devices and software gain wider use, says Muñoz-Avila, GDA agents must be able to recognize and diagnose discrepancies in their environments and take intelligent action. One example is an automated air quality control system programmed to monitor and control a variety of devices. "It is very difficult, if not impossible," he says, "for a programmer to foresee all of the potential situations that such a system will encounter."

Similarly, the openness of many networks requires a cyber security system that can continuously integrate new technologies and services.

"It is not feasible to implement counter measures for all potential threats in advance," he says. "An agent-



based system must continuously monitor the overall network, learn and reason about expectations, and act autonomously when discrepancies are encountered."

THE PRECISE INTERROGATION OF PROTEINS BIOINFORMATICS EXPERT USES GEOMETRY TO MODEL MOLECULAR SURFACES AND SPACES.

View larger illustration >

STORY BY ROBERT W. FISHER '79

AT THIS VERY MOMENT, tens of thousands of proteins are floating in and around the cells of your body. When the right two interact, much like a wrench turning a nut, big things can happen: A cell's energy can be produced, a cell can divide, or a virus can turn a healthy cell to its purposes.

Other times two proteins connect... and nothing happens.

Understanding why some proteins bind and others don't is on the to-do list of biologists around the world. It has also captured the attention of Brian Y. Chen, the P.C. Rossin Assistant Professor of Computer Science and Engineering.

Chen is fond of quoting Stanford University computer scientist Donald Knuth, who once said that biologists "easily have 500 years of exciting problems to work on." Researchers can devote a career to studying just a few of them. The sheer number of possibilities means that it costs a lot of time and money to understand how biological processes work and why they go wrong, to design new drugs, or to detect virus mutations before they become deadly.

The arena of proteins is no less daunting. But what if computers could model the structure and function of proteins and compare them to predict which ones might be the answer to a researcher's question, and which are likely to lead to a dead end?

That's the question that drives Chen's research in structural bioinformatics, the science of making good decisions from vast seas of data about molecular shape and biological systems. "We're trying to interrogate



proteins to determine what they do," says Chen, "in ways that don't require human experts to be on hand for every test. If I can get people as close to the explanation as possible, then they have less experimental work to do."

Chen's results can help researchers answer vexing questions. Why does the chemical switch that tells a cell to divide get stuck in the "on" position, causing a tumor to grow? How does HIV protease find the right spot in DNA to make a cell reproduce the virus? Why does a promising drug stop being effective?

MOVING BEYOND TRIAL AND ERROR

Right now, researchers approach such questions using trial and error. Developing a new cancer drug is one example, says Chen. It can require testing millions of possibilities, and take decades and billions of dollars, while patients continue to suffer and die.

Chen foresees a day when "rational design" will allow scientists to engineer for variations and respond quickly to naturally occurring mutations in proteins. The holy grail is to acquire an understanding of how and why proteins work and an ability to engineer them to do needed functions.

"That's a large and intractable problem to study generally," he says, "so we're taking a lot of baby steps."

Bioinformatics takes data from biological systems and creates mathematical models. "With computing power," says Chen, "we can analyze information at a rate and depth that gives us meaningful results quickly, with a precision that a person can't match."

Chen develops new ways to make computer models reveal not just the fact that there are differences between two structures, but why.

"The computer doesn't know anything about biology, and never will," he says. "Software can select interesting evidence out of an exponential space of possibilities. It is a filtering tool to help experts consider only those possibilities that are relevant."

"We're trying to interrogate proteins to determine what they do in ways that don't require human experts to be on hand for every test." —Brian Chen

Chen's research extends the usefulness of bioinformatics by modeling additional molecular properties, such as the three-dimensional shapes that molecules form, by mapping areas where electrostatic fields are enhanced, and by developing algorithms to compare these features with greater relevance to real-world questions.

"If you can identify the right biochemical properties and incorporate them in the model in realistic ways, then we can offer a representation that is as close to real life as possible," he says.



THE SECRETS IN A SILHOUETTE

One of Chen's current projects extends models that look at the arrangement of atoms in a molecule by precisely representing the 3-D surface of the molecule. Dubbed Volumetric Analysis of Surface Properties, or VASP, this project looks at the silhouettes of the atoms and compares where two molecules overlap and which spaces are unique to one or the other.

Chen pulls up a model of a protein on his computer screen. The image is an irregular and lumpy blob, representing the silhouette of the protein's atoms and their orbiting electrons as well. As he rotates the image on one axis and then on another, a deep, cone-like indentation becomes visible. With the touch of his mouse he can move through the shape in tiny increments, like slices of an MRI scan. As he scrolls he can reveal subtle differences in the shape of the cavity that can be used to tease out small variations from other, related proteins.

"I asked, what would happen if I could cut this shape into tiny cubes?" Chen says. Analyzing the cavities on a subatomic scale reveals more



meaningful results than simply comparing the overall differences in binding sites between two molecules. "There are some cubes that are always the same in every pocket, some that are unique in every pocket, and some that are common to some and different to others," he explains. "It turns out that those regionalized differences can be really significant, and they would get lost in the noise if you just compared overall differences between A and B."

As models recognize increasingly subtle variations, the number of questions biologists have to ask grows exponentially. So Chen created VASP to help narrow down the possibilities.

"For this protein alone there are some 400 variations in the public databases, and it's related to several thousand proteins," Chen says. "So you can imagine thousands of different variations on this pocket, some of which are nearly identical and some very different.

"And this is an easy example."

Here's where Chen and VASP come in. His more granular models of proteins can help researchers better see the similarities between related molecules, such as mutant strains of a disease. In this case, this knowledge can help with the design of new drugs that target commonalities and are thus less susceptible to resistance. By comparing with the entire database of known proteins, "my software can reveal possibilities that reinforce an expert's intuition about what to study, and point out some possibilities they might have overlooked," he says, and it can do so faster and more cheaply than experimental studies.

FINDING MEANING IN EMPTINESS

The leading edge of this research is represented by a collaboration between Chen and Katya Scheinberg, associate professor of industrial and systems engineering. NSF has awarded them nearly half a million dollars to explore a new way of describing binding sites by looking not at the atoms along the boundary but by modeling the empty spaces themselves.

"Looking at the landmarks along the edge works quite well, but aligning the empty space within will allow us to catch additional differences," he says. "It gives a new language for describing how biology can vary."

Chen has also pioneered the exploration of proteins' magnetic attraction. Small electrostatic fields around some of the atoms in a protein "act like tiny magnets" that can enhance or prevent docking with another molecule, Chen says. When these "magnets" along the protein's folds match up with oppositely charged atoms in a binding partner, the bond is strengthened, while opposing magnetic forces can repel proteins that might otherwise be a good fit, he says.

In a phenomenon called electrostatic focusing, the charges within a molecule are larger where the cavities between atoms are smaller. "We've found that some proteins actually make the cavities narrower in order to increase the electrostatic field," Chen says.

DNA molecules use this property to ensure that cell proteins attach at the right spot to correctly imprint instructions. But viruses like HIV exploit this property in an effort to induce a cell to produce more virus instead of normal proteins.

UNION INTERSECTION DIFFERENCE Regionalized differences between protein cavities, says Chen, can

INPUT

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be more significant than overall differences between molecular binding sites.



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Understanding how proteins and viruses navigate DNA "is one of the hardest questions in the field," Chen says. So he is working to develop tools that "help to recognize similarities between a protein and DNA and to pinpoint where they will bond."

With so much data, researchers need clear methods to determine which results to pay attention to and which to ignore.

"There needs to be a number, but you can't just choose it, it has to be extracted from the data," Chen says. He is collaborating with statistician Soutir Bandyopadhyay, assistant professor of mathematics in Lehigh's College of Arts and Sciences, to produce a system that will allow researchers to decide how much similarity or difference is significant enough to warrant a closer look, and then pull only those results from the data.

Bioinformatics is inherently interdisciplinary, so in addition to faculty colleagues Chen involves undergraduate and graduate students from a variety of backgrounds in his research.

"Some of the students in our lab study specific disease proteins, others make mathematical representations of molecular surfaces, and others write software for accelerating comparisons and making them more precise," he says.

Kevin Lee '13, a bioengineering major, spent the summer after graduation working on a conference presentation of his research into a class of proteins called the major histocompatibility complex—molecules responsible for activating appropriate immune response in the body. Lee, who is starting graduate school at Columbia University this fall, is applying VASP algorithms to help predict how well these proteins will bind.

"Being able to classify these proteins will help researchers develop better drug delivery systems for cancers and autoimmune diseases," Lee says. "Using high-performance computing we're able to analyze a huge group of structures at once. It's really revolutionary." Lee initially sought out research in a "wet" biology lab, but was drawn to the promise of using computational tools. "It adds a unique skill set to my repertoire," he says.

"One thing that stands out in Professor Chen's lab is that each student has their own project," Lee says. "He's really put forth effort to help each of us individually, as well as promote collaboration."

Getting conventionally trained scientists to grasp the value of computational tools is one of the big challenges of his field, Chen admits. It's important for him to communicate across the boundaries. "It's exciting when someone whose experience has been mono-disciplinary sees our tools and says, 'Wow, that's incredibly useful, it's not just geeky computer stuff.'"

The common thread between these disparate approaches—representing molecular structure, 3-D shapes and electrostatic forces, and doing statistical analysis—is geometry,

Chen says. An avid computer gamer, he observes that games are broad-brush examples of how geometry is applied to render realistic representations of nature. In his work Chen goes a step further, using geometry to model molecular surfaces and subatomic spaces, and pushing its theories (which are excellent for describing rigid structures) to help understand how flexible molecules move in solution.

"I find all of these things really fascinating, and when they are attached to real biomedical problems, that's

even more exciting," he says. "That's what gets me here early in the morning and keeps me here late."

Jazz, he says, is an apt metaphor for his research.

"In jazz there are always new genres being advanced while others slowly decay," Chen says. "When I see a new direction in which the field can go, that's like a new genre. It's exciting to pick up the melody for a new thing and push it as far as you can go." • Geometric models of molecular surfaces and subatomic spaces shed light on the movement of flexible molecules in solution. Above, Wenjie Yang '13G gives a presentation.



Click or scan the QR code below to see a video about Chen's research.



FEATURE STORY BY AMY WHITE • PHOTOGRAPHY BY RYAN HULVAT

First year of Technical Entrepreneurship master's program yields a crop of new innovators.

Where passion meets opportunity

Imagine taking your idea from spark to reality to market in one year. That's what students do in Lehigh's new master's of engineering in Technical Entrepreneurship (TE) program. Working in studios and labs, students solve problems and develop ideas using creativity methods, then learn to prototype, test markets, form companies and launch businesses.

As they learn, the students explore their ideas and work on projects in teams whose members have diverse skills and interests. Applying new knowledge to their ideas and projects creates a dynamic learning experience and fuels the passion to create.

Matthew Fuchs and Zach Hyder study a patented product in the TE studio classroom while Katelyn Noderer presents a business model (right) and (top right, I-r) Hyder, Deniz Pamukcu, Azim Sonawalla, Randi Tutelman and Devin Greene work with a 3-D printer in the Creativity and Innovation Lab.

The 12-month program graduated its first class in May and of the new degree-holders, 56 percent have formed their own companies, while 37 percent have landed jobs.

Matthew Fuchs says the TE program answered a pull he felt while working in the manufacturing industry after earning his B.S. in mechanical engineering from Lehigh in 2011.

"I realized I wanted to be an entrepreneur," Fuchs says. "I wanted to start my own business. I wanted to innovate and invent." TE provided Fuchs with a place to try out his ideas and gain experience in hands-on product development and practical business formation. As a result, Fuchs started a product development company with two TE classmates after graduation.

"Being in an environment full of other people who are starting their own ventures-that pushes you more," says company co-founder

"There's a big satisfaction

in being able to take

control of your career

and shape it yourself.

this program was one

of the best decisions

-Azim Sonawalla '12, '13G TE

I've made in mv

academic career."

Choosing to go through

Katelyn Noderer, who earned a B.A. in design arts and psychology from Lehigh in 2009 and then served two years in the Peace Corps in Ukraine.

"I wanted to be able to combine those things-design and community involvement," savs Noderer. "To learn how to create a business plan and how to do the financials, and to learn about the kinds of things a regular design degree won't give you. That's what the TE program gave me."

Open to applicants from any undergraduate major, the

program graduated its first class of 14 students in May 2013 and then began educating its second cohort of 28 students. Students come from design and the engineering disciplines; from business majors such as accounting, finance and management; and from liberal arts majors such as journalism, political science, psychology and global studies.

"Innovations, whether new products or intellectual property, are emerging at the confluence of disciplines," says Michael Lehman, professor of practice in the TE program. "TE is where students from different backgrounds who have a passion for innovating collide."

The TE curriculum blends engineering and entrepreneurship, theory and practice, learning and doing, Lehman says. It is designed to encourage and apply students' creativity,

adds Marc de Vinck, the Dexter F. Baker Professor of Practice in Creativity.

"Creativity is just the stepping stone to innovation," says de Vinck. "That's what we need. We don't need iteration. We need lifechanging and world-changing entrepreneurship to happen." TE students have launched ventures and developed products in computer accessories, athletic equipment, fashion, community service, recreation, mobile applications, theater and home health.

While the program is a crucible for students to dream up and launch their own products and companies, it also provides valuable skills for those who want to work for small startups and large corporations, or to be service providers to companies in areas such as accounting and marketing. Recent graduates have landed jobs in construction management, transit technology, building products and pharmaceutical development. Chris Hajjar, who earned a B.S.

> in mechanical engineering from Lehigh in 2012, said his TE training helped him land his job with a drug delivery technologies company.

"The TE program helps you develop a broad spectrum of skills relating to different areas of business," says Hajjar. "That made me an attractive candidate.

"Employers will see you as an asset if you can bring entrepreneurial skills and help build their company."





Click or scan the OR code at left to learn more about Lehigh's Technical Entrepreneurship program.



The master's of engineering (M.Eng.) in Technical Entrepreneurship prepares students to develop ideas into ventures, form companies and bring products to market. The one-year, in-residence program draws on an ecosystem of programs dedicated to business and technology innovation—including Lehigh's Integrated Product Development (IPD) program and its Baker Institute for Entrepreneurship, Creativity and Innovation.

Students come from a variety of undergraduate disciplines. They work individually and in teams to develop and commercialize new products while expanding their skills in creativity, prototyping, visualization, process, team and data management, intellectual property, technology application, and business and economic acumen.

"It's an opportunity for passionate people to create their dream job of helping people solve real problems through technical innovations," says John Ochs, TE program director and professor of mechanical engineering and mechanics. "The result is the creation of new and useful products and services and the launching of their own company-while earning the M.Eng. degree."

Students have access to Lehigh's extensive lab and shop resources, including 3-D rapid prototyping equipment and a TE-dedicated studio classroom and Creativity and Innovation Lab. Faculty teach courses designed exclusively for the program. Students are also connected to a regional community of tech incubation events, resources and organizations. Graduates are equipped to launch their own companies, products and ventures. They also find jobs in new product development with startups and larger companies.

For more information, visit www.lehigh. edu/innovate.



Optimism born of hard limits

Leveraging worst-case scenarios, he strengthens complex networks.

Complex, dynamic networks are found in our cells, in the power grid, and in our financial markets. Nader Motee, assistant professor of mechanical engineering and mechanics, wants to make them more efficient and robust by developing a unified theory of networks that helps engineers build better systems.

The field of network theory burgeoned after World War II, but until about a dozen years ago most models simulated a simple "black box" with an input and an output.

Real-world networks are much more complex, says Motee, who directs Lehigh's Distributed Control and Dynamical Systems (DCDS) Laboratory. "Networks of systems" now model the interconnections and interactions of many black boxes. Motee says. A single short circuit or failed line can cause "cascading failures" that black out huge areas.

And as wind, solar and other renewable power sources come on line, complexity increases. Weather conditions can play havoc with wind and solar from minute to minute. And homes with turbines or solar panels don't just consume electricity—sometimes they sell their excess back to the grid. The added variables make it harder and more time-consuming to adjust the grid.

The solution, says Motee, is more strategic monitoring and control. "If we can partition the network into sub-networks, say 50 across the eastern U.S., and have these bunches of nodes talk to other bunches," he says, controllers can get the right

"It's my job to design a network that works in the worst case, because then it will always work in ordinary situations." —Nader Motee

The nation's power grid contains thousands of generating stations that use coal, gas, nuclear and hydropower to produce and distribute energy to millions of customers. While high-voltage transmission lines shift power across the nation, a vast web of smaller electric lines and transformers deliver consistent current. There are checks

in place to reroute power around failed lines and keep power on.

The grid is feeling stress from soaring power consumption, Motee says. In regional monitoring centers, computers gather feedback from sensors around the grid and provide readouts to engineers who reroute power, often by hand. The volume and complexity of the data means it can require several minutes to resolve an issue.

But it can take just a few seconds for power lines to heat up and melt when they have to compensate for a failure by carrying a failed line's load as well as their own,



information faster and avoid extraneous data.

The DCDS team mathematically models a network's behavior so that worst-case scenarios can be run over and over, until the team is sure its result will work. Ph.D. candidate Milad Siami has proved that power loss in electrical transmission systems has nothing to do with the configuration of the network, but is a function of the properties of individual transmission lines.

Motee has a Young Investigator grant from the U.S. Air Force Office of Scientific Research to study another type of network—unmanned aerial vehicles, or "drones," that fly in formation. This problem highlights the classic tradeoff between performance and stability.

"We have better coordination if every unit can talk to every other, but there is a cost," Motee says. More communication requires more power, which means more batteries, greater weight and limited range for the drones. And increased radio traffic makes the drones easier for an enemy to detect and intercept.

"The challenge is to find the right level of sparsity, so that enough of the right information is exchanged only with the peers that need it, without incurring the cost of unnecessary communications," he says.

Nature is often a model for Motee's work. To get at the vexing question of "hard limits" in complex networks, he is analyzing the glycolysis pathway that produces the adenosine triphosphate (ATP) energy packets cells use for fuel.

The pathway withdraws ATP from the cell's bank of energy packets in order to create more. There has to be enough ATP to initiate the process and make energy available to the rest of the cell; if not, "the cell will crash and die," Motee says.

The electrical grid is subject to the same hard limits. If currents flowing through connected segments get too far out of phase, that part of the grid will crash, no matter how the network is designed or how much redundancy is in place.

In a project funded by the U.S. Office of Naval Research, Motee hopes to prove that cascading failures are the result of this hard limit. "Our team is developing a theory that shows that when there are hard limits, no matter what type of feedback strategies we use to control the networks, there will be critical tradeoffs among performance, robustness and fragility," he says. His goal is to understand the impacts of hard limits in various types of networks and to discover principles that help engineers design "hard limit-free networks."

His work has at least one occupational hazard, Motee says.

"My wife says I'm always thinking of the worst case scenario. It's my job to design a network that works in the worst case, because then it will always work in ordinary situations." **O**

DIDYOUKNOW

Lehigh alumni are engaged in high performance computing and data analytics in a variety of ways. Here are a few examples:



Peg Williams '85 M.S., '87 Ph.D is SVP of high performance computing systems for supercomputer pioneer Cray Inc.



Berk Geveci '96 M.S.,

'00 Ph.D. leads the scientific visualization and informatics teams at Kitware Inc., supporting research in areas such as high performance scientific computing and large data analysis.



Chris Martin '00 is co-founder, CFO and VP for MightyHive, an advertising technology software provider that leverages "Big Data" into real-time online marketing decisions.



David A. Bader

'90, '92G is executive director of high performance computing at Georgia Tech, conducting research at the intersection of high performance computing, computational biology and genomics, and social network analysis.



Nick Kastango '10

mines data for clinical and operational insights at Memorial Sloan-Kettering Cancer Center.

> To learn more about the achievements of Lehigh engineers, visit lehigh.edu/engineering

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LASTING DATA IDENTITY FOR LASTING ACCESS

Robert Kahn, who helped invent the Internet's communications protocols four decades ago, is hard at work today developing repository technology that makes information storage and retrieval more robust.

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