



BIG QUESTIONS IN SCIENCE

CMNS Research Yields Major Discoveries

By Beth Panitz

CMNS RESEARCHERS ARE ON A MISSION. Throughout the college, nearly 1,000 research and tenure-track faculty members, along with their students, are seeking answers to many of science's fundamental questions. "Our dedicated researchers are on the edge of discovery in the never-ending quest for information to add to their discipline's body of knowledge and unlock some of science's biggest mysteries," says CMNS Dean Jayanth Banavar.

That relentless pursuit of scientific breakthroughs is made possible, in part, by the generous support of a host of federal and corporate partners, who last year alone invested more than \$180 million in the college. That investment has yielded strong returns.

On the pages that follow, read more about the big questions CMNS researchers are tackling and the answers they are discovering.

1 What do tiny neutrinos reveal about the universe?

THE THERMOMETER READS -25° F, but that doesn't stop Physics Associate Professor Kara Hoffman from putting on her parka and snow boots and heading into the frigid Antarctic air. While it may be winter break 2012 in College Park, it is summer at the South Pole and prime time for construction on Hoffman's latest experiment. Donning a hard hat, Hoffman helps the crew drill 200 meters into the Antarctic ice to install a unique subsurface telescope covering nearly 100 square kilometers that can detect some of the tiniest particles in our universe—neutrinos.

"Neutrinos are basic building blocks of our universe," says Hoffman. By exploring their properties, she believes, we can learn more about the nature of galaxies and supernovae and unravel astrophysical phenomena occurring millions or even billions of light years away.

Neutral and nearly massless, neutrinos move at light speed and are difficult to detect. They travel from space in straight lines without interacting with anything. In fact, billions of them pass through our bodies unnoticed every second.

Through her work on two NSF-funded projects, Hoffman is expanding our understanding of these tiny particles, which could also tell us more about cosmic rays, high-energy protons that bombard Earth, some having more kinetic energy than a professional baseball pitch. Hoffman notes: "The question is: what could accelerate them to such high energies?" Tracking cosmic rays to find this celestial particle accelerator is elusive because the magnetic field along their path bends the electrically charged particles. But neutrinos offer a clue.

Just as Galileo's optical telescope opened a new lens on space exploration, so do neutrino telescopes. "Galileo studied the heavens by looking at light or photons," notes Hoffman. "Today we can gather different information about the skies by looking for neutrinos."

Hoffman leads the development of the Askaryan Radio Array (ARA), a neutrino



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telescope that uses radio frequency, which transmits best through very cold ice, to detect the particles. Plans are underway for 37 subsurface clusters of radio antennae. In addition, she is a major contributor to the IceCube Neutrino Observatory, completed in 2010, which detects neutrinos inside a cubic kilometer block of ice at the South Pole.

"Whatever produces cosmic rays should also be producing neutrinos," says Hoffman. Traveling in straight lines, their origins are easier to discern. "If we can find some area of the sky where the neutrinos cluster—a twinkling spot of neutrinos—then we can figure out what is accelerating matter to such high energies," says Hoffman. ■

KARA HOFFMAN HELPS WITH THE CONSTRUCTION OF THE ARA NEUTRINO DETECTOR LOCATED NEAR THE SOUTH POLE.



2 Was Einstein correct?

BLACK HOLES may hold the answer to one of science's biggest questions: Does Albert Einstein's theory of general relativity hold true?

"Black holes are places where gravity has gone crazy," says Astronomy Professor Christopher Reynolds, director of the college's Joint Space Science Institute, a partnership with NASA Goddard Space Flight Center. "They have the strongest gravitational fields in the universe. They suck in everything, even light." Those properties make them the perfect natural laboratory to study Einstein's predictions about gravity.

While black holes themselves are undetectable, the super-hot gases spiraling into them emit radiation that can be detected by X-ray telescopes. Reynolds seeks a better understanding of black hole dynamics by examining data from instruments like NASA's Chandra X-ray Observatory and the European Space Agency's X-ray Multi-Mirror Mission (XMM-Newton) that must remain in orbit thousands of miles into space to capture the X-rays.

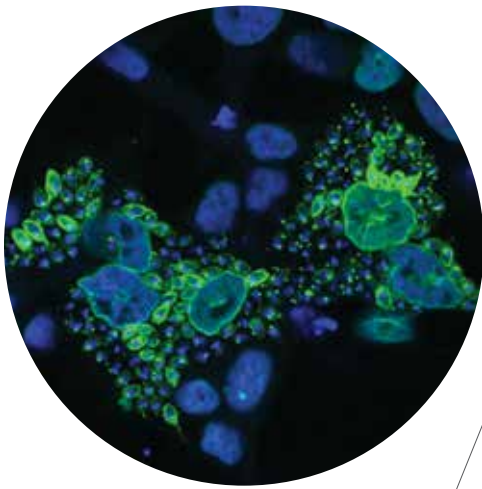
"According to Einstein, space is like a rubber sheet that can bend," says Reynolds. "Black holes can twist the space around them." Using the X-ray telescope observations, Reynolds can calculate how quickly a black hole is rotating and begin to examine this "twisting of space."

Current data supports Einstein's theory, but most scientists predict there is a glitch somewhere.

"There's a disconnection between the two major pillars of physics—general relativity and quantum mechanics. They make fundamentally different assumptions," says Reynolds, whose research is funded by NASA. "Most physicists think Einstein's theory has to give."

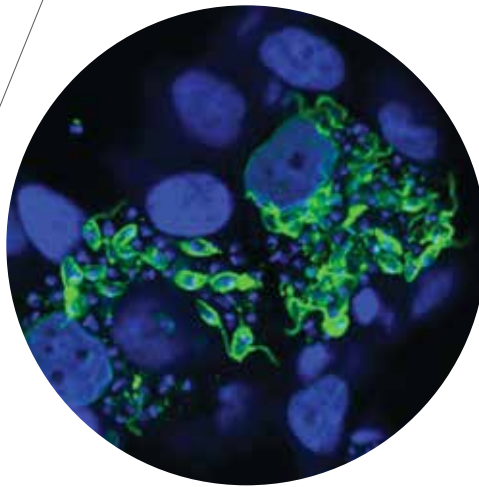
The search for answers is limited by current technology, which collects X-ray light from only a relatively small area and "does not allow us to track changes in the X-ray spectrum of accreting black holes in order to truly test Einstein's assumptions," says Reynolds, who is optimistic that future observatories will shed more light on the mysteries of black holes. He serves as a science advisor for the European Space Agency's proposed Large Observatory for X-ray Timing (LOFT), which is now being considered for construction with a tentative launch around 2020. "With a collection area that's nearly 100 times larger than current observatories, LOFT would enable us to study changes in the spectra of black hole systems in exquisite detail," says Reynolds, "allowing us to conduct new tests of gravity and further our knowledge of how matter interacts with the black hole during its final 'death plunge.'" ■

3 How can deadly pathogens be controlled?



96
HOURS
POST-INFECTION

120
HOURS
POST-INFECTION



**THESE PARASITES
AFFECT SOME
20 MILLION
PEOPLE
WORLDWIDE.**

HUMAN CELLS 96 AND 120 HOURS AFTER INFECTION WITH THE *TRYPANOSOMA CRUZI* PARASITE, WHICH CAUSES CHAGAS DISEASE, EXPRESS A TAGGED FORM OF THE MUCIN-ASSOCIATED SURFACE PROTEINS (MASP), KEY PLAYERS IN THE INFECTION PROCESS. DNA IN BOTH HUMAN CELLS AND PARASITES IS STAINED BLUE.

DEADLY PATHOGENS infecting human cells are all in a day's work for Associate Professor Najib El-Sayed in the Department of Cell Biology and Molecular Genetics and the University of Maryland Institute for Advanced Computer Studies (UMIACS). Under carefully controlled conditions in his campus laboratory, El-Sayed grows three related trypanosomatid parasites that afflict an estimated 20 million people worldwide, causing diseases that run rampant in the developing world, including African sleeping sickness and Chagas disease.

Through his research, El-Sayed exposes these parasites to human cells grown in the laboratory and examines what happens on a genomic level. "We're looking to see how the parasite adapts to the host and how it interferes with the host's defense mechanisms," says El-Sayed, whose research is funded by the National Institute of Allergy and Infectious Diseases of the National Institutes of Health. "Ultimately, our goal is to help scientists develop drug targets or vaccines."

As an undergraduate biology student, El-Sayed was fascinated by parasites. "They have complex, amazing lifecycles that take them from one host to another with incredible ways of modulating the function of every host and changing it to optimize their survival," he notes. That's great for parasites, but it could be lethal for host sites, including humans.

Today, El-Sayed's research utilizes next-generation sequencing technology to follow every single one of a parasite's 10,000 genes and examine how each gene behaves during the infection process. Likewise, he studies how the host cell responds. "We're trying to understand their gene expression programs, which genes turn on and off," he explains.

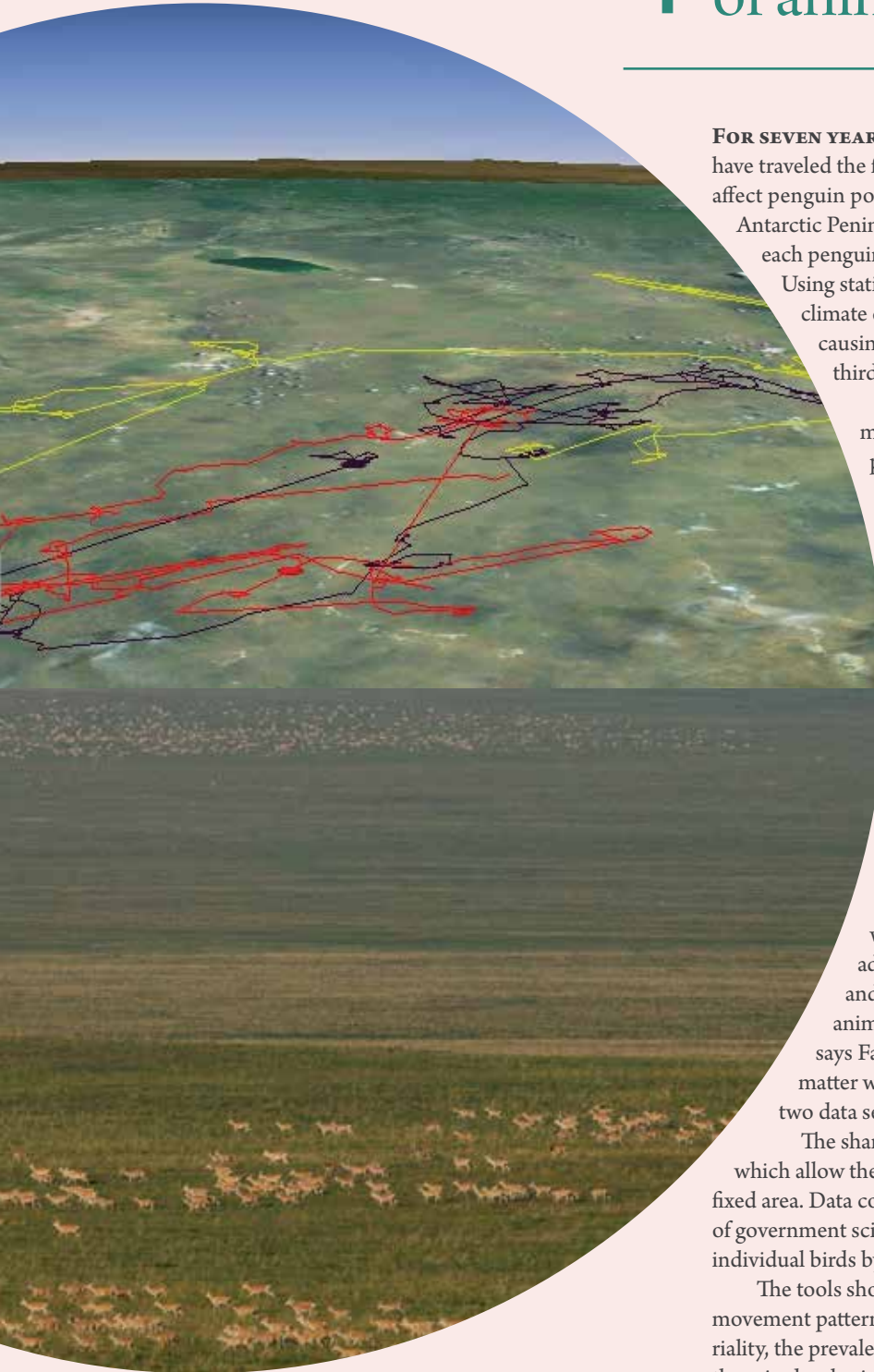
In a major breakthrough, the team recently identified a subset of genes in the Chagas disease-causing *Trypanosoma cruzi* parasite that activates when the pathogen is about to enter the human cell. "That finding tells us these genes must be involved in the infection process," says El-Sayed. Further research indicated that the products of a subset of these genes, the Mucin-Associated

Surface Proteins (MASP), play key roles in the infection process.

Using bioinformatics tools, the researchers then identified a set of proteins in the human host that interacts with MASP. "We theorized that if we could stop that interaction, we could reduce the infection rate of Chagas disease," explains El-Sayed. Spread by the bite of triatomine (kissing) bugs, Chagas disease is a major health problem in South and Central America. Left untreated, about 30 percent of infected individuals develop chronic symptoms, including potentially fatal digestive and heart problems.

Back in the lab, El-Sayed's team has successfully prevented human cells from expressing the pinpointed proteins. "Suddenly the infection rate was reduced dramatically," says El-Sayed, who hopes his work leads to new treatments for a number of life-threatening diseases. "More than one-fifth of the world's population live in areas inhabited by the insects that transmit these parasites," says El-Sayed. "There's a pressing need to find drugs and vaccines for these neglected diseases." ■

4 What drives the movement of animal populations?



FOR SEVEN YEARS, researchers from Biology Professor William Fagan's lab have traveled the frigid Antarctic seas to study how environmental changes affect penguin populations. When their touring vessels stop along the Antarctic Peninsula, the researchers disembark to painstakingly count each penguin and examine their breeding, nesting and feeding patterns. Using statistical and spatial analysis, Fagan's team has concluded that climate change is upsetting long-entrenched penguin dynamics, causing the population of two breeds to dwindle, while a third increases.

Fagan's work meshes field research with theoretical models to study the movement and distribution of animal populations from penguins in Antarctica to gazelles in Mongolia and primates in Panama. The findings help address critical questions in ecology and conservation biology. "To understand the human impact on other species," says Fagan, "we first have to understand how these species use their habitats."

With NSF funding, Fagan is developing a suite of bioinformatics tools to better analyze the movements of animal populations. "There is no one-size-fits-all tool because the data sets can differ greatly," notes Fagan, who is applying the tools to three different case studies: blacktip sharks swimming off Florida's coast, whooping cranes migrating from Wisconsin to Florida and nomadic gazelles traveling up to 1,000 kilometers per year across Mongolian grasslands.

The gazelle study builds off an earlier collaboration with the Smithsonian Institution that tracked the animals adorned with GPS-enabled collars, motion-detecting sensors and satellite uplinks. "Basically, you sit back and wait for the animal to send you an e-mail telling you what it has been up to," says Fagan. The result is a long record of movement data, no matter where the animal travels—quite different than the other two data sets.

The sharks are embedded with radio frequency identification tags, which allow them to be tracked via triangulation as they swim through a fixed area. Data collection on the whooping cranes depends on the efforts of government scientists and birdwatchers across the country who identify individual birds by unique tags.

The tools should help ecologists better understand what drives the movement patterns of a specific population—be it social dynamics, territoriality, the prevalence of predators or the search for resources—and assist them in developing appropriate conservation measures. In the case of the Mongolian gazelles, effective conservation efforts will need to consider the gazelle's nomadic nature, driven by its search for food across highly variable grasslands, says Fagan, who also is associate director of research innovation at SESYNC, the National Socio-Environmental Synthesis Center in Annapolis, a multidisciplinary, five-year, NSF-funded university initiative. ■

5 How do genes change functions in nature?



WHAT DO A FRUIT FLY AND A MOUSE HAVE IN COMMON? More than you might think, says Entomology Professor Leslie Pick, who studies the regulatory genes that control embryo development. In the 1990s, Pick's lab created transgenic fruit flies by inserting a mouse regulatory gene into a fly genome. Using genetic tools, the researchers then expressed the mouse gene in place of the analogous fly gene. "We were amazed that the mouse gene performed a job necessary for the fly's development," says Pick. "We would have thought that the genes for developing a fly—with its cuticle, wings and six legs—would be completely different than those for a mouse."

Pick's experiment and others have changed the way biologists think and led to the launch of a new field called evolutionary developmental biology, or simply "evo-devo." The field explores two of nature's biggest wonders: the development of complex organisms from single-cell embryos and the astonishing diversity of these organisms.

Pick investigates how regulatory genes evolve to allow for this diversity. Encased in a single-celled embryo, regulatory genes act like a set of developmental instructions, controlling the expression of other genes and the cell-differentiation process. Particularly intriguing

is the fact that many of the same regulatory genes appear in very different species.

Pick tracks the evolution of the *ftz* gene, pronounced "futz." "This gene seems to have changed more than some other regulatory genes and now regulates totally different genes than its ancestral form," explains Pick, who conducts the research with NSF funding. "In the fruit fly it regulates segment formation, but in other species it plays a different role. The gene has switched its function somewhere during evolution."

Mysteries abound about this process. "If we made these types of mutations in the lab, the embryo would die," says Pick. The question

remains: How could the genes change in nature without damaging the embryo? Pick predicts: "We will find that evolution works by changing the expression and function of regulatory genes, little bits at a time, that allow the animals to survive and thrive in the wild."

Pick is serving as a rotating program director on evo-devo at NSF until June, while still maintaining her CMNS research projects. "It's been a great opportunity to view the field from a higher level and see how my research fits into the bigger picture." ■

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6 How does energy flow between fast-spinning molecules?

WHEN CHEMISTRY PROFESSOR AMY MULLIN'S RESEARCH on high energy molecules reached an impasse, she did what great scientists have done throughout the ages—developed her own instrumentation to help her seek answers. For years, chemists have investigated how energy flows between molecules, hoping to gain insights into how chemical reactions work, but one type of molecular energy—rotation—has remained elusive. Until Mullin developed a high power optical centrifuge, no tool existed to move enough molecules into the extreme states required for study. Understanding these high-energy molecules could have far-reaching insights into plasma and combustion processes.

The optical centrifuge works by using a special combination of ultrafast laser pulses—called oppositely chirped pulses—to spin molecules into extreme rotational states. “It mimics molecules found under extreme temperature conditions in nature—several thousand degrees Kelvin,” explains Mullin. “But unlike nature, the centrifuge gets the molecules rotating uniformly in space similar to many tiny, spinning gyroscopes. This gives us the potential to control the direction of reactive molecules.”

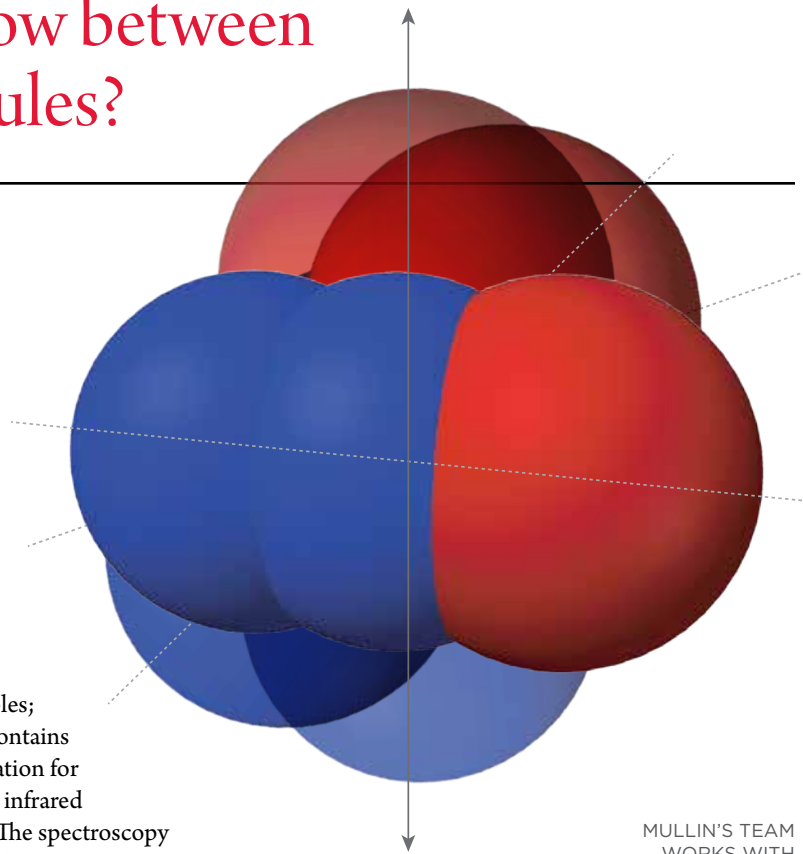
The experiment fills an entire laboratory with its series of contraptions and mechanisms—oscillators, amplifiers, lenses and mirrors—covering three connected tables, encompassing 150 square feet. The centrifuge itself covers

the first two tables; the final third contains the instrumentation for high-resolution infrared spectroscopy. “The spectroscopy allows us to study how the rotational energy is redistributed into other forms of energy through collisions,” says Mullin.

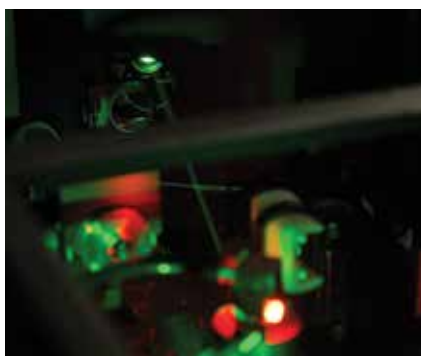
Mullin joined CMNS in 2005 from Boston University with the dream of building this revolutionary tool. Despite naysayers in the scientific community, Mullin designed, built and began operating the centrifuge in four years. The working instrumentation wowed NSF, which granted Mullin funding to continue the project.

Her research is just beginning to yield insights into the dynamics at play in these molecules. “What’s surprising,” says Mullin, “is that once we get the molecules spinning,

the spin persists even after several thousand collisions. Then it goes into translational energy.” With varied molecular compounds behaving somewhat differently, Mullin’s graduate and undergraduate student team members have their work cut out for them. “We have to take a lot of measurements to sort out the general from the specific,” says Mullin. “But we have already sparked the imagination of many chemists and physicists by showing that we can put these molecules into extreme states.” ■



MULLIN'S TEAM WORKS WITH SPINNING N₂O MOLECULES.



PHOTOS FROM LEFT: PRECISION OPTICS RECOMBINE OPTICAL CENTRIFUGE PULSES. THE GREEN LIGHT AMPLIFIES THE POWER OF THE PULSES. THE EXTREME ROTATIONAL STATES OF N₂O ARE CREATED AND PROBED IN A LOW PRESSURE CELL.

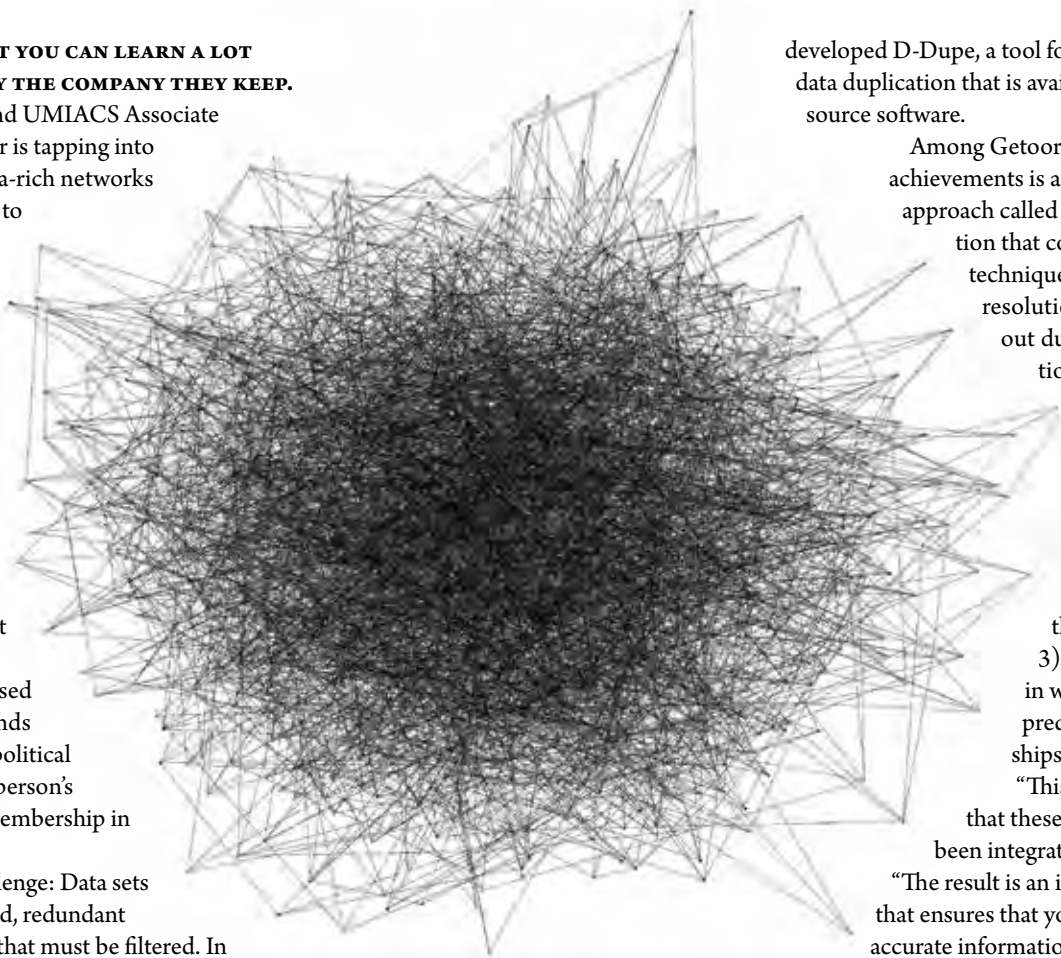
7 How can artificial intelligence decipher complex data?

IT'S BEEN SAID THAT YOU CAN LEARN A LOT ABOUT SOMEONE BY THE COMPANY THEY KEEP.

Computer Science and UMIACS Associate Professor Lise Getoor is tapping into the abundance of data-rich networks and using computers to understand and analyze that relational information and how it can be applied. For example, biologists can infer a protein's cellular function by examining its relationships in a protein-to-protein interaction network. Marketers can predict whether someone will buy a product based on whether their friends have bought it. And political scientists can infer a person's views by analyzing membership in online groups.

The biggest challenge: Data sets are frequently jumbled, redundant and filled with noise that must be filtered. In 2000, Getoor's doctoral research launched a new area of artificial intelligence called "statistical relational machine learning," which combines statistical approaches with relational machine learning strategies to make sense out of messy data sets. Today, her research is funded by a range of government agencies, including NSF and the Defense Advanced Research Projects Agency, and technology giants Google, Microsoft and Yahoo!

Another common problem: inconsistencies in data sets. "How do you figure out whether two similar references refer to the same entity?" Getoor poses. For example, in bibliographic information, do J. Smith, Jonathan Smith and John Smith all refer to the same person? Getoor has developed "entity resolution" strategies that tackle this problem by examining relational information. If J. Smith and Jonathan Smith have several co-authors in common, they more likely are the same entity. Getoor and her students have developed new algorithms that make use of relational information and other contextual information to improve the accuracy of entity resolution. With fellow researchers at the university's Human-Computer Interaction Laboratory, Getoor



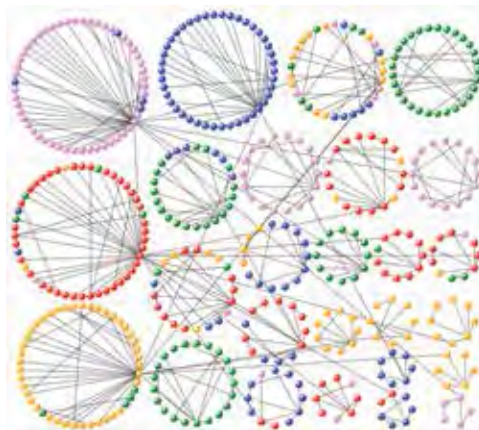
developed D-Dupe, a tool for eliminating data duplication that is available as open-source software.

Among Getoor's crowning achievements is a data-cleaning approach called graph identification that combines three techniques: 1) entity resolution, which weeds out duplicate information, 2) collective classification, where nodes are identified and labeled based on their relationship with other nodes in the network and 3) link prediction, in which the model predicts relationships between data.

"This is the first time that these strategies have been integrated," says Getoor.

"The result is an improved model that ensures that you have more accurate information." Getoor plans

to apply her algorithms to specific areas, including personalized medicine in which extensive data sets can be used to tailor medical treatment to each patient's individual characteristics. ■



GRAPH IDENTIFICATION TRANSFORMS COMPLEX DATA SETS (ABOVE) INTO DATA APPROPRIATE FOR FURTHER ANALYSIS (LEFT).

8 Why do continents exist only on planet Earth?

DISTINGUISHED UNIVERSITY PROFESSOR AND GEOLOGY DEPARTMENT CHAIR ROBERTA RUDNICK is trying to crack a mystery that lies far beneath the ground we walk on. Rudnick studies the evolution of the Earth's continental crust. "Interestingly, none of the other planets in our solar system have continents," she points out. "Understanding continent formation can broaden our knowledge about many processes on Earth, including our own species' evolution."

Geologists agree that the continental crust formed when magma melted in the Earth's mantle, erupting to the surface. "The perplexing thing is that the continental crust is comprised of rocks that could not have come directly from the Earth's mantle," says Rudnick, "so other processes must have been involved." The crust has an andesitic bulk composition, while geologists would expect it to have a basaltic composition, like the Earth's oceanic crust and terrestrial areas on Mars and Venus. This "Crust Composition Conundrum" puzzles Rudnick, and she has traveled the globe for answers.

Her research currently takes her to Eastern China, where she looks for clues in rock samples brought to the surface through volcanic eruptions—what Rudnick calls a poor man's drill hole. "We would love to drill down and collect samples, but it's hugely expensive, and is not feasible past 12 kilometers," says

Rudnick, who explains that the base of the crust is 40 kilometers deep and the underlying lithosphere is 150 kilometers below the Earth's surface.

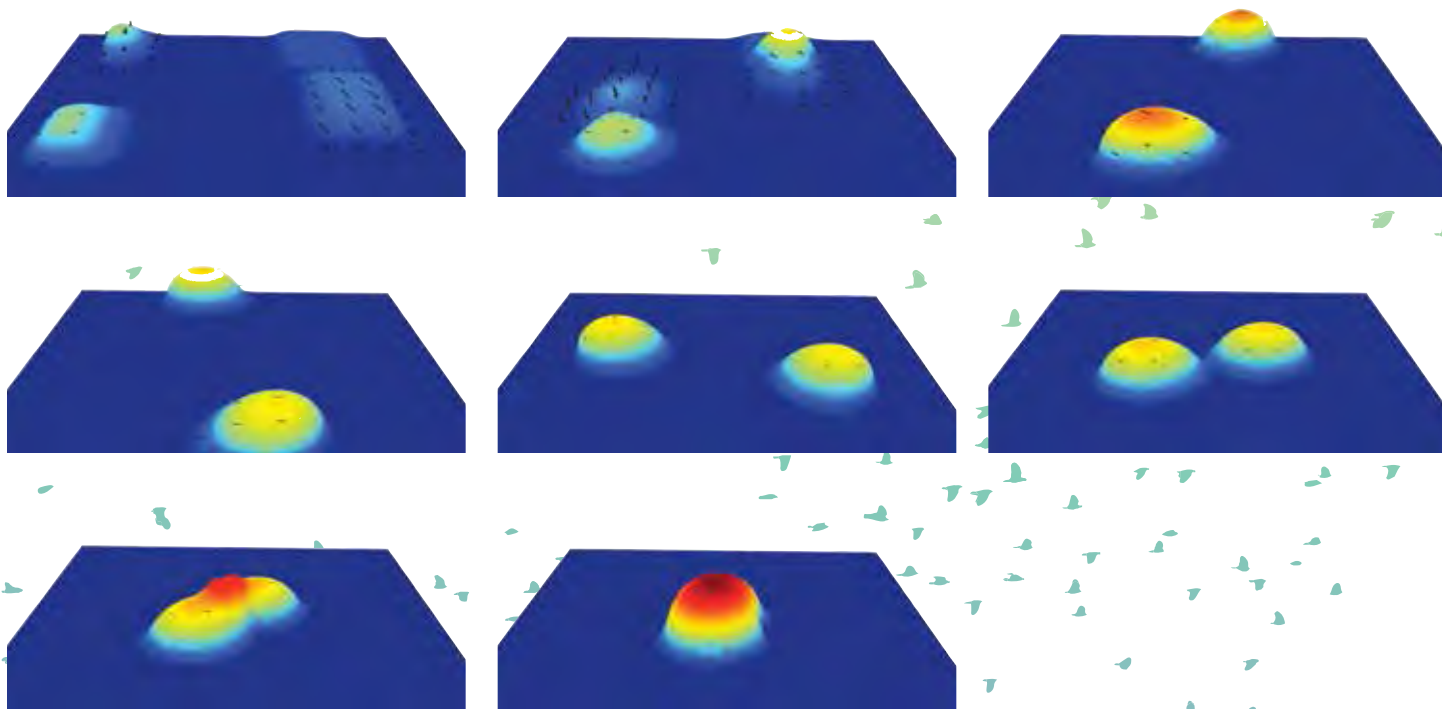
Back in the campus geochemical laboratories, her research team has analyzed the samples extensively, finding evidence to explain the conundrum. One theory, called "recycling of the lower crust," posits that millions of years ago the crust was basaltic, but that over time the denser minerals, containing iron and magnesium, accumulated in the lower crust and eventually sank into the mantle. Her lab also unearthed evidence that chemical weathering has changed the crust composition over the ages by removing soluble elements, such as magnesium.

Rudnick, an elected member of the National Academy of Sciences, is also reassessing the continental crust composition to derive a better estimate of its radioactive elements. In the past year, she and her collaborators have traveled to Central China, South Africa, Namibia, Canada, as well as Idaho and Wyoming, to collect samples from glacial tillites—rock material deposited during ice ages throughout history. The information could help uncover further mysteries of continent evolution, including how weathering of continents responded to the rise of atmospheric oxygen some 2.4 billion years ago. ■



ROBERTA RUDNICK EXAMINES AND LABELS MANTLE XENOLITHS WITH GRADUATE STUDENT JINGAO LIU AT YANGYUAN, SHANXI PROVINCE, CHINA.

9 How do mathematical models explain nature?



KONSTANTINA TRIVISA SEES MATHEMATICS IN PLAY EVERYWHERE SHE LOOKS, whether it's a flock of birds flying overhead, a school of fish in a stream, the ocean's waves or the blood flowing through our veins. The mathematics professor applies her expertise in nonlinear partial differential equations to model complex physical systems and to prove how existing models apply to specific phenomena. "I'm not the type of mathematician who develops an idea simply because it's beautiful mathematics," says Trivisa. "I always have an application in mind that would interest an engineer, physicist or biologist."

Take the example of biologists studying the dynamics of flocking birds. Using traditional "particle systems," the research is computationally expensive and time consuming. "With my collaborators, I constructed a model that captures the relevant phenomena,

including unpredictable events, such as the presence of wind. This model can greatly reduce the computational cost of investigation," says Trivisa.

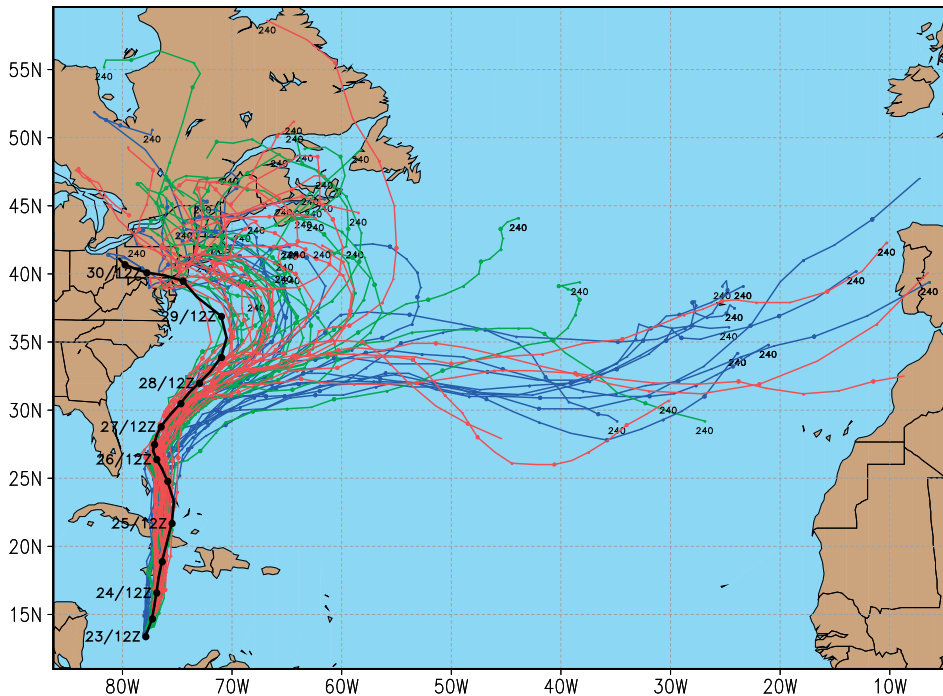
Much of Trivisa's research focuses on developing the mathematical methods to better understand fluid dynamics, materials science and phase transition processes. She received a prestigious NSF Presidential Early CAREER Award for her work, and plans to apply her mathematical skills, using a fluid dynamics and mechanics approach, to biomedical issues. She is beginning to investigate fluid-structure interaction in blood flow, which is relevant for the design of cardiovascular treatments, such as stents used to improve the flow through narrow or weak arteries.

A native of Greece, Trivisa moved to the United States in 1991 for her doctoral studies. She joined CMNS in 2000 and currently directs the interdisciplinary Applied Mathematics, Statistics, and Scientific Computation Program and is an affiliate professor in the Institute of Physical Science and Technology. "Working with a large community of scientists and engineers keeps me focused on the big questions in science," says Trivisa, who continues to foster scientific collaborations in which she can apply mathematics to provide key answers. ■

VISUALIZATION ABOVE SHOWS THE EVOLUTION OF FOUR DISTINCT FLOCKS OF BIRDS: AS TIME PASSES, THE BIRDS APPROACH EACH OTHER AND FINALLY MERGE TO ONE FLOCK AS PREDICTED BY THE MODEL.

10

How can we improve weather forecasting?



NCEP-GFS ENSEMBLE FORECASTS OF HURRICANE SANDY

BLUE 12Z OCT 23, 2012
GREEN 18Z OCT 23, 2012
RED 00Z OCT 24, 2012
BLACK SANDY'S ACTUAL TRACK

IT MAY HAVE BEEN ONE OF THE BIGGEST NATURAL DISASTERS to strike the East Coast, but Superstorm Sandy was also a scientific triumph of numerical weather prediction, says Distinguished University Professor Eugenia Kalnay, a world-renowned expert in numerical weather prediction (NWP) in the Department of Atmospheric and Oceanic Science. “I’m quite impressed by the operational forecasts of Sandy,” she says. “The precipitation, the winds and even the estimation of the uncertainty of the forecasts—they were all impressively accurate.”

This accuracy is due, in part, to Kalnay’s own work over the past 30 years. At the National Weather Service (NWS) from 1987 to 1997, she headed the research division that develops the computer atmospheric models and the methods for “assimilating observations” used for forecasting the weather. “Our seven-day forecast is now about as accurate as a one or two-day forecast was in the 1960s,” she notes. Still, weather prediction is difficult as evidenced by the storm that started in Iowa on June 29, 2012, and evolved into a “derecho” that moved eastward for more than 12 hours with very severe weather all the way to the Washington, D.C. region, leaving

behind widespread devastation and power outages. Although the NWS Storm Prediction Center issued severe thunderstorm warnings along the route, further improvements in NWP means future warnings could be provided days, not hours, in advance.

One of the keys to improving weather forecasts is to ensure that atmospheric computer models start with an accurate estimate of current atmospheric conditions. As an expert on “data assimilation,” Kalnay develops methods to better determine initial conditions generated from observations, such as satellite and radar information. Researchers and students worldwide use her book, *Atmospheric Modeling, Data Assimilation and Predictability*, which has been translated into Chinese and Korean.

Kalnay and Distinguished University Professor James Yorke founded the college’s Weather & Chaos group, which has made groundbreaking improvements in data assimilation systems and numerical weather prediction, graduating some 20 doctoral experts in the process. Kalnay is also a pioneer in ensemble forecasting, a technique that she developed and implemented operationally 20 years ago at the NWS. “Instead of making a

single forecast, we use slightly different initial conditions and create an ensemble of 20 forecasts,” she explains. “This way, we can predict forecast uncertainty by examining where these weather forecasts agree or disagree, making them much more useful.” The introduction of this information extended forecasts from three to seven days beginning in the mid 1990s.

More recently, the ensemble approach has been combined with data assimilation in the Local Ensemble Transform Kalman Filter, a method developed by Brian Hunt, a professor in the Weather & Chaos group, and adopted by several countries for operational weather prediction. In the future, the approaches could have other important applications as well. “The ideas of ensemble prediction and data assimilation could be adopted to improve forecasts of other types, such as economic forecasts,” adds Kalnay. ■

