SCIENCE NEWS

Capturing the Energy of Slow Motion

A new concept in energy harvesting could capture energy that is currently mostly wasted due to its characteristic low frequency and use it to power next-generation electronic devices. In a project funded by electronics giant Samsung, a team of Penn State materials scientists and electrical engineers has designed a mechanical energy transducer based on flexible organic ionic diodes that points toward a new direction in scalable energy harvesting of unused mechanical energy in the environment, including wind, ocean waves and human motion.

Devices to harvest ambient mechanical energy to convert to electricity are widely used to power wearable electronics, biomedical devices and the so-called Internet of Things (IoT) — everyday objects that wirelessly connect to the internet. The most common of these devices, based on the piezoelectric effect, operate most efficiently at high frequency, greater than 10 vibrations per second. But at lower frequencies their performance falls off dramatically.

"Our concept is to specifically design a way to turn low-frequency motion, such as human movement or ocean waves, into electricity," said *Qing Wang*, professor of materials science and engineering, Penn State. "That's why we came up with this organic polymer p-n junction device."

Called an ionic diode, their device is composed of two nanocomposite electrodes with oppositely charged mobile ions separated by a polycarbonate membrane. The electrodes are a polymeric matrix filled with carbon nanotubes and infused with ionic liquids. The nanotubes enhance the conductivity and mechanical strength of the electrodes. When a mechanical force is applied, the ions diffuse across the membrane, creating a continuous direct current. At the same time, a built-in potential that opposes ion diffusion is established until equilibrium is reached. The complete cycle operates at a frequency of one-tenth Hertz, or once every 10 seconds.

For smart phones, the mechanical energy involved in touching the screen could be converted into electricity that can be stored in the battery. Other human motion could provide the energy to power a tablet or wearable device.

"Because the device is a polymer, it is both flexible and lightweight," Wang said. "When incorporated into a next-generation smart phone, we hope to provide 40 per cent of the energy required of the battery. With less demand on the battery, the safety issue should be resolved."

According to the authors on the paper "Flexible Ionic Devices for Low-Frequency Mechanical Energy Harvesting" published online in the journal *Advanced Energy Materials,* "The peak power density of our device is in general larger than or comparable to those of piezoelectric generators operated at their most efficient frequencies."

Michael Hickner, associate professor of materials science and engineering, produced the ionic polymers, with Liang Zhu, a postdoctoral scholar in his group. Qiming Zhang, distinguished professor of electrical engineering, and his group focused on device integration and performance. Wang's group, including coauthors postdoctoral scholar Qi Li and graduate student Yong Zhang, focused on materials optimisation. The co-lead authors are visiting scholar Ying Hou, recent Ph.D graduate Yue Zhou and visiting scholar Lu Yang, all part of Zhang's group.

"Right now, at low frequencies, no other device can outperform this one. That's why I think this concept is exciting," Wang said.

Climate Change Is already Causing Widespread Local Extinction in Plant and Animal Species

Extinctions related to climate change have already happened in hundreds of plant and animal species around the world. New research, to be published in the open-access journal *PLOS Biology,* shows that local extinctions have already occurred in 47 per cent of the 976 plant and animal species studied.

Climate change is predicted to threaten many species with extinction, but determining how species will respond in the future is difficult. Dozens of studies have already demonstrated that species are shifting their geographic ranges over time as the climate warms, towards cooler habitats at higher elevations and latitudes. The new study, by Professor John J. Wiens from the University of Arizona, used these range-shift studies to show that local extinctions have already happened in the warmest parts of the ranges of more than 450 plant and animal species. This result is particularly striking because global warming has increased mean temperatures by less than 1 degree Celsius so far. These extinctions will almost certainly become much more widespread over time, because temperatures are predicted to increase by an additional 1 to 5 degrees in the next several decades. These local extinctions could also extend to species that humans depend on for food and resources.

The study also tested the frequency of local extinction across different regions, habitats, and groups of organisms. It found that local extinctions occurred in about half of the species surveyed across different habitats and taxonomic groups. However, the results showed that local extinctions varied by region and were almost twice as common among tropical species as among temperate species. This is important as the majority of plant and animal species live in the tropics. The results of this study contribute to our understanding of how plants and animals will respond to global climate change and highlight the need to slow and prevent further warming.

Computers Can Take Social Media Data and Make Marketing Personas

Computers may be able to group consumers into marketing segments in real time just by observing how they respond to online videos and other social media data, according to a team of researchers.

In a study, computers used information from social media accounts to automatically build marketing personas, said James Jansen, professor of information sciences and technology, Penn State. Marketing research professionals typically create these personas to help editors and marketers better understand the behaviors of specific consumer groups, he added.

"A lot of times we have to use numbers in decision making, whether that's using numbers in understanding a market segment or an audience base or demographics, for instance," said Jansen. "But it's hard to make a decision looking at a bunch of complex numbers that most people don't understand. One way that has been proposed and implemented in a wide number of domains to understand consumers is through personas. Researchers take a bunch of market data and condense it into a fictitious person."

Marketers, who create personas manually with data from focus groups, ethnography methods and surveys, can then hold conversations and make decisions based on these personas.

"The problem with that, though, is that, in addition to being time consuming and expensive, they can rapidly become obsolete," said Jansen.

Computer-drawn personas, on the other hand, not only can be created in real time and at relatively low costs, but they can be updated quickly as economic conditions and demographics continue to change.

The researchers developed algorithms to analyse data, such as demographic information, topics of interest and customer interactions, from 188,000 subscribers of a news website. The data included the subscribers' YouTube profiles, which included demographic information such as gender, age and country location, and their interactions with videos on the site, such as the topics of videos watched by the users.

This site had posted approximately 2,807 videos to its YouTube channel that were viewed by 30 million users in 217 countries.

The algorithms then identified unique ways that groups of people were interacting with the information, in this case, news videos.

News site editors could use this information to better collect and target content to these audiences, said Jansen, who worked with Haewoon Kwak, research scientist and Jisun An, postdoctoral researcher, both of Qatar Computing Research Institute, Hamad Bin Khalifa University.

"Journalists want to have a better understanding of just who their actual users are," said Jansen. "They can use that information to reach readers with better titles, content and article framing."

While the researchers used news and information in this study, the technology could be applied to other types of consumer transactions, according to the researchers, who presented their findings at the Second International Workshop on Online Social Networks Technologies held in Agadir, Morocco.

"The method is transferrable to other domains," said Jansen. "It could work at any consumer touchpoint — any place where we can see what the consumers are buying or what they are viewing before they buy and then tie it back to some demographics."

Jansen said the technology is also scalable and could use other types of social media to analyze consumer behavior and create marketing personas.

"We're now scaling this up to millions of users," he said. "And we could use other types of social media data, from Facebook or Twitter, for example."

Electron-photon Small-talk Could Have Big Impact on Quantum Computing

In a step that brings silicon-based quantum computers closer to reality, researchers at Princeton University have built a device in which a single electron can pass its quantum information to a particle of light. The particle of light, or photon, can then act as a messenger to carry the information to other electrons, creating connections that form the circuits of a quantum computer.

The research, published in the journal *Science* and conducted at Princeton and HRL Laboratories in Malibu, California, represents a more than five-year effort to build a robust capability for an electron to talk to a photon, said Jason Petta, a Princeton professor of physics.

"Just like in human interactions, to have good communication a number of things need to work out — it helps to speak the same language and so forth," Petta said. "We are able to bring the energy of the electronic state into resonance with the light particle, so that the two can talk to each other."

The discovery will help the researchers use light to link individual electrons, which act as the bits, or smallest units of data, in a quantum computer. Quantum computers are advanced devices that, when realised, will be able to perform advanced calculations using tiny particles such as electrons, which follow quantum rules rather than the physical laws of the everyday world.

Each bit in an everyday computer can have a value of a 0 or a 1. Quantum bits — known as qubits — can be in a state of 0, 1, or both a 0 and a 1 simultaneously. This superposition, as it is known, enables quantum computers to tackle complex questions that today's computers cannot solve.

Simple quantum computers have already been made using trapped ions and superconductors, but technical challenges have slowed the development of silicon-based quantum devices. Silicon is a highly attractive material because it is inexpensive and is already widely used in today's smartphones and computers.

The researchers trapped both an electron and a photon in the device, then adjusted the energy of the electron in such a way that the quantum information could transfer to the photon. This coupling enables the photon to carry the information from one qubit to another located up to a centimetre away.

Quantum information is extremely fragile — it can be lost entirely due to the slightest disturbance from the environment. Photons are more robust against disruption and can potentially carry quantum information not just from qubit to qubit in a quantum computer circuit but also between quantum chips via cables.

For these two very different types of particles to talk to each other, however, researchers had to build a device that provided the right environment. First, Peter Deelman at HRL Laboratories, a corporate research-and-development laboratory owned by the Boeing Company and General Motors, fabricated the semiconductor chip from layers of silicon and silicon-germanium. This structure trapped a single layer of electrons below the surface of the chip. Next, researchers at Princeton laid tiny wires, each just a fraction of the width of a human hair, across the top of the device. These nanometer-sized wires allowed the researchers to deliver voltages that created an energy landscape capable of trapping a single electron, confining it in a region of the silicon called a double quantum dot.

The researchers used those same wires to adjust the energy level of the trapped electron to match that of the photon, which is trapped in a superconducting cavity that is fabricated on top of the silicon wafer.

Prior to this discovery, semiconductor qubits could only be coupled to neighboring qubits. By using light to couple qubits, it may be feasible to pass information between qubits at opposite ends of a chip.

The electron's quantum information consists of nothing more than the location of the electron in one of two energy pockets in the double quantum dot. The electron can occupy one or the other pocket, or both simultaneously. By controlling the voltages applied to the device, the researchers can control which pocket the electron occupies.

"We now have the ability to actually transmit the quantum state to a photon confined in the cavity," said Xiao Mi, a graduate student in Princeton's Department of Physics and first author on the paper. "This has never been done before in a semiconductor device because the quantum state was lost before it could transfer its information."

The success of the device is due to a new circuit design that brings the wires closer to the qubit and reduces interference from other sources of electromagnetic radiation. To reduce this noise, the researchers put in filters that remove extraneous signals from the wires that lead to the device. The metal wires also shield the qubit. As a result, the qubits are 100 to 1000 times less noisy than the ones used in previous experiments.

Eventually the researchers plan to extend the device to work with an intrinsic property of the electron known as its spin. "In the long run we want systems where spin and charge are coupled together to make a spin qubit that can be electrically controlled," Petta said. "We've shown we can coherently couple an electron to light, and that is an important step toward coupling spin to light."

Mathematical Algorithms Calculate Social Behaviour

For a long time, mathematical modelling of social systems and dynamics was considered in the realm of science fiction. But predicting, and at once influencing human behaviour is well on its way to becoming reality. Scientists at the Technical University of Munich (TUM) are currently developing the appropriate tools. This will allow them to simulate and improve security at major events or increase the efficiency of evacuation measures.

There is a long history of research aimed at predicting the behaviour of groups and influencing them. But, it seems practically impossible to precisely predict the behaviour of individuals, not least because of the myriad interactions between the physical, emotional, cognitive and social domains.

But things look quite different when considering people in traffic, in social networks and at major events in which they do not appear as individuals, but rather as part of a crowd. "People in masses behave akin to particles in a fluid or gas," explains Professor Massimo Fornasier, chair of the Department of Applied Numerical Analysis at TU Munich.

Analogy to Physics

In physics, it is not necessary to know the properties of every individual particle to calculate with a high probability the direction of flow of a large number of gas molecules. It is enough to understand their mean motion properties.

"We can take the same approach when looking at flows of human masses, animal swarms or interacting robots: Analogous to the force of attraction between molecules in a gas, we can describe generalised behavioural patterns as resulting from interacting social forces between individual agents and represent them in mathematical equations," says Fornasier, describing his approach.

Calculating Collective Behavioural Patterns

Professor Fornasier and his team have recently proven mathematical statements that demonstrate how surprisingly easy it is to automatically generate precise models for specific, relatively simple group interactions based on observed dynamics data.

Using computer simulations, the mathematicians can describe potential collective behavioural patterns of a large number of individuals who mutually influence each other in a given situation. "In the next step we can then also make predictions about future behaviour," says Fornasier. "And once we can calculate the behaviour of a group of interacting agents in advance, we are only one small step away from controlling them."

Informed Agents Follow the "Herd Instinct"

In an experiment conducted in May 2015 in collaboration with Consiglio Nazionale delle Ricerche (CNR) and the University of Rome 'La Sapienza' in Italy, Fornasier and his team demonstrated that the process is in fact amenable to influencing group behaviour.

To this end, the researchers assigned two groups of 40 students each the task of finding a specific location in a building. The scientists planted two incognito informed agents into one of the groups. By merely moving very determinedly in a predefined direction, the agents were able to steer the group toward the target spot.

This experiment demonstrates that taking control of self-organising systems, which also include groups of individuals, is possible with surprisingly little effort. The mathematicians also confirmed that the results apply equally well to very large groups. "In fact, two to three agents per 100 individuals are sufficient," says Massimo Fornasier.

Herding Dog Strategy for Opinion Forming

The fact that his mathematical models are formulated in an entirely abstract environment makes them easily adaptable to a wide variety of situations. This facilitates finding efficient solutions for steering large masses of people through buildings in a stress-free manner or evacuating people in emergency situations.

"But we can also apply our results to other interesting domains in society, like the behaviour of investors in financial markets," says Fornasier. There, precisely coordinated activities by big investors can result in sizable market movements.

Opinion forming in groups also builds on the interactions of people. In their models, the mathematicians demonstrated that it is most effective to concentrate on the most radical defenders of a given opinion. If you manage to convince them, the rest of the group will follow.

"There is also a good model for this in nature," according to Fornasier. "To drive a herd of sheep in a desired direction, a good herding dog will always concentrate on the animal that is the farthest removed from the group. They achieve their goal by reining in the most stubborn animal."

Limits of Prediction

"For all the conceivably good application scenarios there remains, of course, the question of abuse," says Professor Fornasier. "The good news in this context is that we have also proven that behaviour is not so easy to predict or control for all kinds of dynamics and situations."

"An important prerequisite for predictability and controllability is that the myriad possible interactions between the agents in a large group can be reduced to a small number of effective ones," says Massimo Fornasier. "Forecasts function well in groups that show generalised patterns of behaviour."

However, with competing interactions, when the energy of individual agents is too large an equilibrium and, thus, concerted movement of the group of agents can no longer be imposed using simple, sporadic interventions.

"An extensive forecast of events like that accomplished by the mathematician Hari Seldon in Isaac Asimov's Foundation series or the all-encompassing control exercised in Aldous Huxley's 'Brave New World' will remain science fiction," says Professor Fornasier.

Mimicking Biological Movements with Soft Robots

Designing a soft robot to move organically — to bend like a finger or twist like a wrist — has always been a process of trial and error. Now, researchers from the Harvard John A. Paulson School of Engineering and Applied Sciences and the Wyss Institute for Biologically Inspired Engineering have developed a method to automatically design soft actuators based on the desired movement.

The research is published in *The Proceedings of the National Academy of Sciences.*

"Rather than designing these actuators empirically, we wanted a tool where you could plug in a motion and it would tell you how to design the actuator to achieve that motion," said Katia Bertoldi, the John L. Loeb Associate Professor of the Natural Sciences and coauthor of the paper.

Designing a soft robot that can bend like a finger or knee may seem simple but the motion is actually incredibly complex.

"The design is so complicated because one actuator type is not enough to produce complex motions," said Fionnuala Connolly, a graduate student at SEAS and first author of the paper. "You need a sequence of actuator segments, each performing a different motion and you want to actuate them using a single input."

The method developed by the team uses mathematical modeling of fluid-powered, fiber-reinforced actuators to optimise the design of an actuator to perform a certain motion. The team used this model to design a soft robot that bends like an index finger and twists like a thumb when powered by a single pressure source.

"This research streamlines the process of designing soft robots that can perform complex movements," said Conor Walsh, the John L. Loeb Associate Professor of Engineering and Applied Sciences, Core Faculty Member at the Wyss Institute for Biologically Inspired Engineering and coauthor of the paper. "It can be used to design a robot arm that moves along a certain path or a wearable robot that assists with motion of a limb."

The new methodology will be included in the Soft Robotic Toolkit, an online, open-source resource developed at SEAS to assist researchers, educators and budding innovators to design, fabricate, model, characterise and control their own soft robots.

Mind-controlled Toys: The Next Generation of Christmas Presents?

The next generation of toys could be controlled by the power of the mind, thanks to research by the University of Warwick.

Led by Professor Christopher James, Director of Warwick Engineering in Biomedicine at the School of Engineering, technology has been developed which allows electronic devices to be activated using electrical impulses from brain waves, by connecting our thoughts to computerised systems.

Some of the most popular toys on children's lists to Santa — such as remote-controlled cars and helicopters, toy robots and Scalextric racing sets — could all be controlled via a headset, using 'the power of thought'.

This could be based on levels of concentration — thinking of your favourite colour or stroking your dog, for example.

Instead of a hand-held controller, a headset is used to create a brain-computer interface — a communication link between the human brain and the computerised device. Sensors in the headset measure the electrical impulses from brain at various different frequencies — each frequency can be somewhat controlled, under special circumstances. This activity is then processed by a computer, amplified and fed into the electrical circuit of the electronic toy.

Professor James comments on the future potenti al for this technology: "Whilst brain-computer interfaces already exist — there are already a few gaming headsets on the market — their functionality has been quite limited. New research is making the headsets now read cleaner and stronger signals than ever before — this means stronger links to the toy, game or action thus making it a very immersive experience.

"The exciting bit is what comes next — how long before we start unlocking the front door or answering the phone through brain-computer interfaces?"

New Classes of Electron Orbits Discovered

Phenomena like solar flares and auroras are consequences of magnetic reconnection in the near-earth space. These "magnetic reconnection" events are akin to magnetic explosions that accelerate particles as they rapidly change the topology of the magnetic field lines. Researchers in Japan have used a new Particle-In-Cell (PIC) simulator to understand how magnetic reconnection works for the tenuous plasma surrounding our earth and have identified new classes of electron orbits that help scientists understand the characteristics of the fast jets of electrons that stream from the reconnection region. The researchers explain their results this week in *Physics of Plasmas,* from AIP Publishing.

The ionized gas in space, called 'plasma,' is so tenuous that the charged particles (ions and electrons) rarely collide with each other, but move in very complex ways due to the electric and magnetic fields. This process is highly nonlinear because as the electrons move, they carry the electric current which in turn changes the electromagnetic field. The self-consistent nonlinear motion of the particles and of the electromagnetic field is a complex system that is hard to predict.

"We investigate basic mechanisms of magnetic reconnection in tenuous space plasma, by using a computer simulation that allows us to solve both the electromagnetic fields and the motions of virtual plasma particles," said Seiji Zenitani, a scientist at the National Astronomical Observatory of Japan. Although PIC simulations are widely used and can solve the motion of virtual particles, often all the particle trajectories are not checked. The reason is two-fold: on the one hand, because PIC simulation generates very large data sets; on the other, because until now, scientists had thought that all the basic orbits were already discovered in the 1980s. By comprehensively scanning the simulation data, the research team was careful not to overlook anything.

While this approach is straightforward for a small collection of particles, as a result of an extensive survey of PIC simulation with nearly two billion particles, researchers were able to identify several new classes of electron orbits.

"We were surprised to find 'noncrossing electron orbits' that do not cross the midplane, a finding contrary to conventional belief that all the particles cross the midplane ($z=0$) during magnetic reconnection," Zenitani said. So, while it is a standard strategy to track electron trajectories from the midplane, by definition, this does not work for the noncrossing electrons. Analysis suggests that the noncrossing electrons are the majority, at least in the number density. The particle orbits are fundamental elements for the kinetic physics of magnetic reconnection which could lead to the revision of theoretical models.

"In addition, NASA's Magnetospheric Multiscale (MMS) mission observes the electron properties in and around near-earth reconnection sites now," Zenitani said. "Our results provide hints that will help to better interpret MMS data."

New Evidence Shows How Bacterium in Undercooked Chicken Causes Guillain-Barre Syndrome

A Michigan State University research team is the first to show how a common bacterium found in improperly cooked chicken causes Guillain-Barre Syndrome, or GBS.

The federally funded research, now published in the *Journal of Autoimmunity*, not only demonstrates how this food-borne bacterium, known as Campylobacter jejuni, triggers GBS, but offers new information for a cure.

If chicken isn't cooked to the proper minimum internal temperature, bacteria can still exist.

"What our work has told us is that it takes a certain genetic makeup combined with a certain Campylobacter strain to cause this disease," said Linda Mansfield, lead author and MSU College of Veterinary Medicine professor. "The concerning thing is that many of these strains are resistant to antibiotics and our work shows that treatment with some antibiotics could actually make the disease worse."

GBS is the world's leading cause of acute neuromuscular paralysis in humans and despite much speculation, the exact mechanisms of how this autoimmune disease develops have been widely unknown.

"We have successfully produced three preclinical models of GBS that represent two different forms of the syndrome seen in humans," Mansfield said. "Our models now provide a unique opportunity to understand how your personal genetic type may make you more susceptible to certain forms of GBS."

Another area of concern more recently among scientists is related to an increase of the disease due to the Zika virus. Mansfield said there are many other bacteria and viruses associated with GBS and her models and data could be useful in studying these suspected causes, as well as finding better treatment and prevention options.

Despite the severity of GBS, treatments have been very limited and fail in many cases. In fact, the use of certain antibiotics in Mansfield's study aggravated neurological signs, lesions and the number of immune antibodies that can mistakenly attack a patient's own organs and tissues.

"These models hold great potential for discovery of new treatments for this paralysis," Mansfield said. "Many patients with GBS are critically ill and they can't participate in clinical trials. The models we identified can help solve this."

Those suffering from GBS can initially experience vomiting and diarrhea, but can often write the symptoms off as eating bad food. One to three weeks later, they can begin to develop weakness and tingling in the feet and legs. Gradually, paralysis can spread to the upper body and arms, and even a respirator may be needed for breathing.

Mansfield now wants to move forward quickly to test drugs against GBS in her models.

"Of course new treatments would be wonderful," she said, "but therapeutics to prevent GBS from developing in the first place would be the best strategy so that people don't have to suffer with paralysis."

Campylobacter jejuni infects more than a million people yearly in the United States and is also known to trigger other autoimmune disorders such as Inflammatory Bowel Disease and Reiter's arthritis.

New Way to Trap Dangerous Gases

A team of researchers at the University of Texas at Dallas has developed a novel method for trapping potentially harmful gases within microscopic organo-metallic structures.

These metal organic frameworks, or MOFs, are made of different building blocks composed of metal ion centers and organic linker molecules. Together they form a honeycomb-like structure that can trap gases within each comb, or pore.

The tiny nano-scale structures also have the potential to trap various emissions from things as immense as coal factories and as small as cars and trucks. However, there are some molecules that are simply too weakly adsorbed to remain contained within the MOF scaffolding. Adsorption describes how an extremely thin layer of molecules (as of gases, solutes or liquids) can cling to the surfaces of solid bodies or liquids.

"These structures have the ability to store gases, but some gases are too weakly bound and cannot be trapped for any substantial length of time," said Dr. Kui Tan, a research scientist in the Department of Materials Science and Engineering at UT Dallas and lead author of the study published online in *Nature Communications.*

After studying this problem, Tan decided to try to introduce a molecule that can cap the outer surface of each MOF crystal in the same way bees seal their honeycombs with wax to keep the honey from spilling out.

In this case, Tan introduced vapors of a molecule called ethylenediamine, or EDA, that created a monolayer, effectively sealing the MOF "honeycomb" and trapping gases such as carbon dioxide, sulfur dioxide and nitric oxide within.

This monolayer is less than 1 nanometer in thickness, or less than half the size of a single strand of DNA.

To quantify how much gas was trapped and remained in the EDA-capped MOF structures, Tan and his team used time-resolved, in-situ infrared spectroscopy, testing the efficiency of this molecular "cork" to trap weakly adsorbed gases.

The presence of the gas molecules adsorbed in the MOF was displayed on a nearby computer screen as inverted peaks, which revealed that EDA vapor was able to effectively retain the greenhouse gas carbon dioxide for up to a day.

"Potential applications of this finding could include storage and release of hydrogen or natural gas to run your car, or in industrial uses where the frameworks could trap and separate dangerous gases to keep them from entering the atmosphere," Tan said.

As an added discovery, Tan found that a mild exposure to water vapor would disrupt the monolayer, penetrate the framework and fully release the entrapped vapors at room temperature. Such selectivity of the EDA membrane opens up new options for managing gas emissions, he said.

"The idea of using EDA as a cap came from Kui who proceeded to do an enormous amount of work to demonstrate this new concept, with critical theoretical input from our collaborators at Wake Forest University," said Dr. Yves Chabal, head of the materials science and engineering department in the Erik Jonsson School of Engineering and Computer Science and senior author of the paper.

Predicting Extinction, with the Help of a Yule Tree

At this time of year, the words "Yule tree" may conjure images of brightly decorated balsam firs. But for Lea Popovic, an Associate Professor of Mathematics and Statistics in the Faculty of Arts and Science, a Yule tree is actually an advanced way to describe evolution.

In a new study published in *Mathematical Biology,* Popovic and recent Concordia graduate Mariolys Rivas (PhD 14) show how the present-day distribution of physical traits across species can help explain how the evolutionary process unfolded over time.

They used a tree-shaped graph called the Yule tree, first developed in 1924 by G. U. Yule to map genealogical history.

Visualising How Species Change

"The full history of the evolutionary process of a given species can be neatly described by a Yule tree," says Popovic.

"We extended Yule's model so that we would be able to track evolutionary processes that are dependent on specific phenotypes."

Reconstructing the evolutionary process has been a major challenge to scientists for decades because so much is unknown. And with increased planetary changes resulting in growing numbers of extinctions, these questions are even more pressing.

"The evolution of the visible traits of species — their phenotypes — is responsible for the diversity of all living organisms and for their ability to adapt to new environments," says Popovic.

"Recent research has shown how differences in phenotypes can affect how quickly species evolve or become extinct. Mathematical models can go a long way in helping us determine various elements of this process. But the possibility that diversification may be trait dependent implies that standard methods are not adequate for measuring the rates of evolution."

To address these concerns, Popovic and Rivas used math to map the rate at which new species are created or become extinct. They developed a new mathematical model that describes evolution as a process in which the length of time that species live until they go extinct — or give rise to other species — depends on their phenotype. Their model includes the possibility for the phenotype of the new species to change.

The Yule Tree Graph

The Yule tree is a graph with one edge coming in and two edges coming out of each branch-point. The branches represent the time periods between the evolution of new species. If the branch leads to a branch-point, it means a new species evolved. If the branch leads to a leaf, it marks an extinction. The leaves represent the species present today.

The graph also features "cherries," which represent two present species that are the closest to each other in evolutionary terms, and "pendants," which represent the evolutionary connection to another species that is slightly further from them in evolutionary terms.

Counting the number of different types of cherries and pendants helps determine the particular dependence on the phenotype of new species being created or going extinct.

Researchers Watch Biomolecules at Work

Scientists at the University of Bonn have succeeded in observing an important cell protein at work. To do this, they used a method that allows to measure structural changes within complex molecules. The further developed procedure makes it possible to elucidate such processes in the cell, i.e., in the natural environment. The researchers are also providing a tool kit, which allows a wide range of molecules to be measured. Their study has now been published in the journal *Angewandte Chemie International Edition.*

If we want to open a Christmas season walnut, we usually use a nutcracker. In the simplest case, this consists of two arms, which move against each other around a joint and can thus exert pressure on the shell. Very simple, actually — to understand how this kind of nutcracker works, it is sufficient for us to see it in action just once.

However, it is much more difficult to understand how cellular molecules work. They also alter their spatial structure as they work — similar to the nutcracker, where the arms open or close. These conformational changes tell experts a great deal about the way in which the molecule fulfills its job. Unfortunately, it is very difficult to measure these kind of movements because they occur on a very small length scale. This applies even more so if one wants to investigate the structural changes in the natural cellular environment, where countless simultaneous processes make it very hard to isolate any specific information from the general noise.

The working group from the Institute for Physical and Theoretical Chemistry at the University of Bonn has now succeeded in doing this. To this end, the scientists further developed a method that has been used for many years to measure distances within large molecules. "However, this normally only works in a test tube," explains the head of the study, Professor Olav Schiemann.
"In contrast, our technique can also be used in cells."

The researchers used what is known as electron paramagnetic resonance spectroscopy (EPR) for their measurements. The molecule to be measured is usually given a magnetic marker at two different sites. Through radiation with microwaves, the polarity of one of these mini magnets is reversed. The magnetic field emitted by it is thus changed, which in turn influences the second mini magnet. This influence is greater the closer both markers are to each other.

"We now measure how strongly the second magnet reacts to the reverse polarity of the first," explains Schiemann. "From this, we can ascertain the distance between both markers." If — metaphorically speaking — both arms of the nutcracker are marked in this way, their movement against each other can be understood.

Magnetic Ruler Measurements

In principle, the technique is not new. "However, we have succeeded in producing a new kind of label with which we can mark a wide range of biomolecules in a site-specific way," explains Schiemann's staff member Jean Jacques Jassoy. Usually, these labels consist of radicals — which are chemical compounds that carry a single free electron. The electron acts as a magnet during the measurement. The problem here: single electrons are highly reactive — they try to form pairs of electrons as quickly as possible. The chemists at the University of Bonn thus used a very stable radical in their work — a so called trityl group. They created various derivatives of this trityl radical. Each of these magnetic markers is designed to target specific sites within biomolecules and thus enables several approaches for the structural analysis of different biomolecules.

In their study, the researchers used this methodological advance to investigate a protein from the cytochrome P450 group. These proteins occur in almost all living beings and fulfill important tasks, for instance during oxidation processes in the cell. "With our method, we were able to precisely measure the distance between two areas of the cytochrome to a fraction of a millionth of a millimeter," emphasises Schiemann's staff member Andreas Berndhäuser.

The procedure is suitable for making biomolecule conformational changes visible in the cell. At the same time, it also generally facilitates the clarification of molecular structures. Schiemann: "We are thus providing researchers with a new tool kit that could help answer many biochemical questions."

Smallest Transistor Ever

A research team led by faculty scientist Ali Javey at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) has done just that by creating a transistor with a working 1-nanometer gate. For comparison, a strand of human hair is about 50,000 nanometers thick

"We made the smallest transistor reported to date," said Javey, lead principal Investigator of the Electronic Materials program in Berkeley Lab's Materials Science Division. "The gate length is considered a defining dimension of the transistor. We demonstrated a 1-nanometer-gate transistor, showing that with the choice of proper materials, there is a lot more room to shrink our electronics."

The key was to use carbon nanotubes and molybdenum disulfide (M_0S_2), an engine lubricant commonly sold in auto parts shops. MoS, is part of a family of materials with immense potential for applications in LEDs, lasers, nanoscale transistors, solar cells, and more.

The findings were published today in the journal *Science*. Other investigators on this paper include Jeff Bokor, a faculty senior scientist at Berkeley Lab and a Professor at UC Berkeley: Chenming Hu, a Professor at UC Berkeley: Moon Kim, a Professor at the University of Texas at Dallas; and H.S. Philip Wong, a Professor at Stanford University.

The development could be key to keeping alive Intel co-founder Gordon Moore's prediction that the density of transistors on integrated circuits would double every two years, enabling the increased performance of our laptops, mobile phones, televisions, and other electronics.

"The semiconductor industry has long assumed that any gate below 5-nanometers wouldn't work, so anything below that was not even considered," said study lead author Sujay Desai, a graduate student in Javey's lab. "This research shows that sub-5-nanometer gates should not be discounted. Industry has been squeesing every last bit of capability out of silicon. By changing the material from silicon to M_0S_2,, we can make a transistor with a gate that is just 1 nanometer in length, and operate it like a switch"

When 'electrons are out of control'

Transistors consist of three terminals: a source, a drain, and a gate. Current flows from the source to the drain, and that flow is controlled by the gate, which switches on and off in response to the voltage applied.

Both silicon and M_0S_2, have a crystalline lattice structure, but electrons flowing through silicon are lighter and encounter less resistance compared with M_0S_2,. That is a boon when the gate is 5-nanometers or longer. But below that length, a quantum mechanical phenomenon called tunneling kicks in, and the gate barrier is no longer able to keep the electrons from barging through from the source to the drain terminals.

"This means we can't turn off the transistors," said Desai. "The electrons are out of control."

Because electrons flowing through M_0S_2 are heavier, their flow can be controlled with smaller gate lengths. M_0S_2can also be scaled down to atomically thin sheets, about 0.65 nanometers thick, with a lower dielectric constant, a measure reflecting the ability of a material to store energy in an electric field. Both of these properties, in addition to the mass of the electron, help improve the control of the flow of current inside the transistor when the gate length is reduced to 1 nanometer.

Once they settled on M_0S_2 as the semiconductor material, it was time to construct the gate. Making a 1-nanometer structure, it turns out, is no small feat. Conventional lithography techniques don't work well at that scale, so the researchers turned to carbon nanotubes, hollow cylindrical tubes with diameters as small as 1 nanometer.

They then measured the electrical properties of the devices to show that the M_0S_2 transistor with the carbon-nanotube gate effectively controlled the flow of electrons.

"This work demonstrated the shortest transistor ever," said Javey, who is also a UC Berkeley Professor of electrical engineering and computer sciences. "However, it's a proof of concept. We have not yet packed these transistors onto a chip, and we haven't done this billions of times over. We also have not developed self-aligned fabrication schemes for reducing parasitic resistances in the device. But this work is important to show that we are no longer limited to a 5-nanometer gate for our transistors. Moore's Law can continue a while longer by proper engineering of the semiconductor material and device architecture."

The work at Berkeley Lab was primarily funded by the Department of Energy's Basic Energy Sciences program.

The Incredible Shrinking Particle Accelerator

Long valued for their role in scientific discovery and in medical and industrial applications such as cancer treatment, food sterilisation and drug development, particle accelerators, unfortunately, occupy a lot of space and carry hefty price tags. The Large Hadron Collider at CERN in France and Switzerland, for example — the world's largest and most powerful particle accelerator — has a circumference of 17 miles and cost $10 billion to build. Even smaller accelerators, such as those used in medical centers for proton therapy, need large spaces to accommodate the hardware, power supplies and radiation shielding. Such treatment facilities typically fill a city block and cost hundreds of millions of dollars to build.

But efforts are under way to make this technology more affordable and accessible by shrinking both the size and the cost without losing the capability. One of the most exciting developments is the plasma accelerator, which uses lasers or particle beams rather than radio-frequency waves to generate the accelerating field. Researchers have already shown the potential for laser plasma acceleration to yield significantly more-compact accelerators. But further development is needed before these devices — envisioned as almost literally "tabletop" in many applications — make their way into everyday use.

This is where advanced visualisation tools and supercomputers such as the Edison and Cori supercomputers at Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center (NERSC) come in.

"To take full advantage of the societal benefits of particle accelerators, game-changing improvements are needed in the size and cost of accelerators, and plasma-based particle accelerators stand apart in their potential for these improvements," said Jean-Luc Vay, a senior physicist in Berkeley Lab's Accelerator Technology and Applied Physics Division (ATAP).

Vay is leading a particle accelerator modeling project as part of the NESAP program at NERSC and is the principal investigator on one of the new exascale computing projects sponsored by the U.S. Department of Energy (DOE). "Turning this from a promising technology into a mainstream scientific tool depends critically on large-scale, high-performance, high-fidelity modeling of complex processes that develop over a wide range of space and time scales," he said.

Vay and a team of mathematicians, computer scientists and physicists are working to do just that by developing software tools that can facilitate simulating, analyzing and visualising the increasingly large datasets produced during particle accelerator studies.

Accelerator modeling is an opportunity to help lead the way to exascale applications, noted ATAP Division Director Wim Leemans. "We've spent years preparing for this opportunity," he said, pointing to the already widespread use of modeling in accelerator design and the tradition of collaboration between physics and computing experts that has been a hallmark of ATAP's modeling work.

"One of the driving factors in our research is the transition to exascale and how data visualisation is changing," explained Burlen Loring, a computer systems engineer who is part of the collaboration, along with Oliver Rübel, David Grote, Remi Lehe, Stepan Bulanov and Wes Bethel, all of Berkeley Lab, and Henri Vincenti, a Berkeley Lab postdoctoral researcher from CEA in

France. "With exascale systems, traditional visualisation becomes prohibitive as the simulation get larger and the machines get larger — storing all the data doesn't work and the file systems and data bandwidth rates aren't keeping up with the compute capacity."

In-Situ to the Rescue

Now, in a paper published in *IEEE Computer Graphics and Applications* (IEEE CG&A), the team describes a new approach to this challenge: WarpIV. WarpIV is a plasma and accelerator simulation, data visualisation and analysis toolkit that marries two software tools already widely used in high energy physics: Warp, an advanced particle-in-cell simulation framework, and VisIt, a 3D scientific visualisation application that supports most common visualisation techniques. Together, they give users the ability to perform *in-situ* visualisation and analysis of their particle accelerator simulations at scale — that is, while the simulations are still running and using the same high performance computing resources — thus reducing memory usage and saving computer time.

"We have this push to transition a significant portion of our visualisation work over to the in situ domain," Loring said. "This work is a step in that direction. It is our first take on in situ for laser plasma accelerators and our first chance to use it on a real science problem."

A primary function of WarpIV is to manage and control the end-to-end, integrated simulation and in situ visualisation and analysis workflow. To achieve this, WarpIV supports four main modes of operation — batch, monitoring, interactive and prompt — each of which in turn supports a different approach to in situ scientific discovery. WarpIV also uses a factory pattern design to define simulation models, which allows users to create new simulation and in situ analysis models in a self-contained fashion; and Python-based visualisation and analysis scripts.

"One of the design factors that will make it easy for scientists to use WarpIV is the ability to use Python scripts that are autogenerated in VisIt," Loring explained. "The scientist takes a representative dataset before they make their runs and comes up with visualisation scripts. Then they open the representative dataset in VisIt and use the recording feature to automatically record their actions into a Python script. Then WarpIV takes these scripts and runs them in the in situ environment."

Another key feature of WarpIV is its integrated analytics — notably, filtered particle species, which enable users to pick out particular features of interest from the hundreds of millions of particles required for accurate simulation.

"Very often when you do a visualisation, particularly in situ, you want to minimize how much time you spend on it, and you can do this by focusing on particular features," Rübel explained. "In this case, for example, you need large numbers of particles to simulate the process, but the features you are interested in, such as the beam that is extracted from the background plasma, are going to be much smaller than that. So finding these features and doing the analysis while the simulation is running, this is what we call filtered species. It is a mechanism we developed not just to do plots, but to find what it is you want to plot."

Towards 3D Modeling

WarpIV, which Rübel initially prototyped in 2013, grew out of a collaboration between two

DOE SciDAC projects: SDAV (Scalable Data Management, Analysis and Visualisation) and COMPASS (Community Project for Accelerator Science and Simulation) programs. The work was also subsequently supported by DOE's CAMPA (Consortium for Advanced Modeling of Particle Accelerators) program.

The WarpIV toolkit, which continues to undergo development, was officially rolled out in June 2016 and is available via bitbucket. Initial testing has yielded positive results in terms of scalability, performance, usability and proven impact on science.

For example, in the research that resulted in the IEEE CG&A paper, the team ran a series of ion accelerator simulations in 2D and 3D to analyse WarpIV's performance and scalability. Comparison of these simulations revealed significant quantitative differences between the 2D and 3D models, highlighting the critical need for high-resolution 3D simulations in conjunction with advanced in situ visualisation and analysis to enable the accurate modeling and study of new breeds of particle accelerators.

In one 3D series, they tracked the run time for five categories of operations at 50-iteration simulation updates and found that, at each update, the visualisation, analysis and I/O operations consumed 11–15 per cent of the total time, while the rest was used by the simulation — a ratio the researchers consider "quite reasonable." They also found that the in situ approach reduced the I/O cost by a factor of more than 4000x.

There is great demand for 3D simulation codes that run in a reasonable time and perform accurate accelerator modeling with correct quantitative predictive power, Vay emphasised.

"We want to be able to conduct experiments on ion acceleration, so in this case it is very important to have a working simulation tool to predict and analyse all kinds of experiments and test theories," said Bulanov, a research scientist in the Berkeley Lab Laser Accelerator Center who works closely with Vay. "And if the simulations can't keep pace with the experiment, it would slow us down significantly."

Having in situ tools like WarpIV will be increasingly valuable as supercomputers transition to more complex manycore architectures, Vay added.

"WarpIV provides visualisation in 3D that we would not have been able to obtain easily using our previous visualisation tools, which were not scaling as well to many computational cores," he said.

World's Smallest Radio Receiver Has Building Blocks the Size of Two Atoms

Researchers from the Harvard John A. Paulson School of Engineering and Applied Sciences have made the world's smallest radio receiver — built out of an assembly of atomic-scale defects in pink diamonds.

This tiny radio — whose building blocks are the size of two atoms — can withstand extremely harsh environments and is biocompatible, meaning it could work anywhere from a probe on Venus to a pacemaker in a human heart.

The research was led by Marko Loncar, the Tiantsai Lin Professor of Electrical Engineering at SEAS, and his graduate student Linbo Shao and published in *Physical Review Applied.*

The radio uses tiny imperfections in diamonds called nitrogen-vacancy (NV) centers. To make NV centers, researchers replace one carbon atom in a diamond crystal with a nitrogen atom and remove a neighboring atom — creating a system that is essentially a nitrogen atom with a hole next to it. NV centers can be used to emit single photons or detect very weak magnetic fields. They have photoluminescent properties, meaning they can convert information into light, making them powerful and promising systems for quantum computing, phontonics and sensing.

Radios have five basic components — a power source, a receiver, a transducer to convert the high-frequency electromagnetic signal in the air to a low-frequency current, speaker or headphones to convert the current to sound and a tuner.

In the Harvard device, electrons in diamond NV centers are powered, or pumped, by green light emitted from a laser. These electrons are sensitive to electromagnetic fields, including the waves used in FM radio, for example. When NV center receives radio waves it converts them and emits the audio signal as red light. A common photodiode converts that light into a current, which is then converted to sound through a simple speaker or headphone.

An electromagnet creates a strong magnetic field around the diamond, which can be used to change the radio station, tuning the receiving frequency of the NV centers.

Shao and Loncar used billions of NV centers in order to boost the signal, but the radio works with a single NV center, emitting one photon at a time, rather than a stream of light.

The radio is extremely resilient, thanks to the inherent strength of diamond. The team successfully played music at 350 degrees Celsius — about 660 Fahrenheit.

"Diamonds have these unique properties," said Loncar. "This radio would be able to operate in space, in harsh environments and even the human body, as diamonds are biocompatible."

This research was coauthored by Mian Zhang, Matthew Markham and Andrew M. Edmonds. It was supported in part by the STC Center for Integrated Quantum Materials.