



Sciencia

BREAKING BOUNDARIES IN PHYSICS & TECHNOLOGY

HIGHLIGHTS:

- Improving Cancer Treatment with Nanomedicine
- CART: Pointing the Way to Reliable Robotic Assistants
- Taking the Sting Out of Big Data
- The Thorium Isomer: Paving the Way for Nuclear Clocks

EXCLUSIVES:

- CERN
- The Virgo Interferometer

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WELCOME...

In this exciting edition of Scientia, we showcase some of the latest discoveries and innovations across the interconnected fields of engineering, technology and the physical sciences.

To begin, our opening section celebrates scientists and engineers behind recent breakthroughs in medical technology. As COVID-19 continues to wreak havoc across the globe, decades of innovation in medical technology have enabled clinicians to save countless lives during this devastating pandemic.

From models that predict viral spread, to software that allows us to work from home, computing is also at the forefront of our fight against COVID-19. Therefore, the next section features researchers who harness computing and data science to tackle a variety of challenges – from protecting online privacy, to optimising treatment guidelines for patients with chronic conditions.

Our third section introduces researchers working across diverse fields of engineering – from those developing sophisticated robotic assistants to those creating new technology that can predict natural disasters.

Next, we report on some exciting developments in the critical field of materials science. In this penultimate section, we meet scientists who are developing new materials for advanced technologies – from nanoparticles for efficient solar cells, to organic coatings that protect metal from costly corrosion.

Our final section of this edition showcases the latest physics research, with a deep dive into the nuts and bolts of our physical reality. Here, we highlight a variety of fascinating projects, each dedicated to unravelling how matter behaves at its most fundamental level, while also laying the foundation for revolutionary new technologies.



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Published in the UK, by
Science Diffusion Ltd

ISSN 2059-8971 (print)
ISSN 2059-898X (online)

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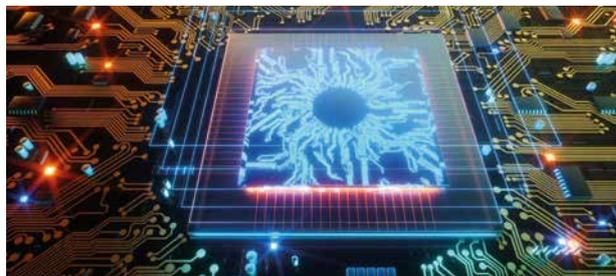
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MEDICAL TECHNOLOGY





SAVING LIVES THROUGH INNOVATIONS IN MEDICAL TECHNOLOGY

From rapid diagnostic kits to life-saving respirators, medical technology is at the forefront of our fight against COVID-19. While the virus is a formidable foe, decades of innovations have allowed us to save countless lives during this devastating global pandemic.

To celebrate these great advances, our opening section of the edition is dedicated to some of the latest research in medical technology and its implementation – from cancer diagnostics and treatment, to helping the law protect patients who rely on medical devices to stay healthy.

In the first article of this section, we meet Dr Baowei Fei from the University of Texas at Dallas, who is pioneering an innovative new technique to detect prostate cancer more accurately than ever before. Combining positron emission tomography with ultrasound, Dr Fei's diagnostic technology can allow prostate cancer to be detected at an

early stage, increasing survival rates and greatly improving patient outcomes.

Next up is Dr Afsaneh Lavasanifar and her research group at the University of Alberta, who aim to improve cancer treatment through the use of nanotechnology. By delivering drug-loaded nanoparticles directly to tumour tissues, the team's approach improves the effectiveness of cancer drugs while reducing their side-effects.

From here, we shift our focus to technology that improves the health of patients with paraplegia. As people with paraplegia are unable to walk, the lack of activity and loading causes the legs to lose strength, while bones reduce in density, leading to a much higher chance of fractures. Therefore, a team of researchers at the University of Reading have developed a new technology involving electrical stimulation and gaming to prevent long-term decline in bone and muscle.

In our next article, we highlight the research of Dr Nigel Shrive at the University of Calgary, who explores innovative new ways to assess and treat various medical conditions, paying particular attention to the heart and joints. By looking at heart and joint problems through the lens of engineering mechanics, his research is improving the lives of people who suffer from mechanical failure within the body.

Our final article of this section explores legal issues faced by people who have attached or implanted medical devices. As these technologies increase in complexity, lawmakers are struggling to keep up, with potentially devastating consequences for the millions of people who rely on medical devices to stay alive and healthy. Here, we introduce Professor Muireann Quigley at the University of Birmingham, whose research team is working hard to bring law, regulation, and policy regarding these technologies into the 21st century.

A NEW TECHNIQUE FOR TARGETED PROSTATE CANCER BIOPSIES

Two-dimensional transrectal ultrasound (TRUS) guided biopsy is the standard method for prostate cancer diagnosis. However, the technique is limited in one respect – it can be prone to sampling error. Cancers can be missed, or their severity grossly underestimated. To address this, **Dr Baowei Fei**, from the University of Texas (UT) at Dallas and UT Southwestern Medical Center, is pioneering a technique that merges positron emission tomography (PET) with TRUS to detect prostate cancer more accurately than before.

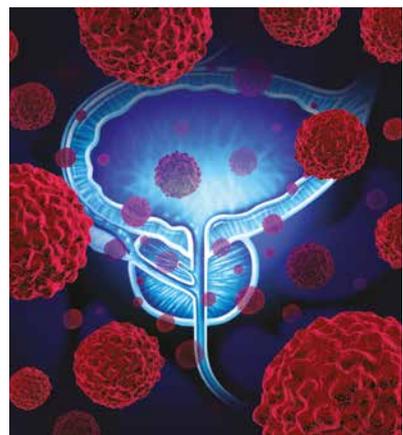
Detecting Prostate Cancer

Prostate cancer is one of the most common types of cancer – it affects some one million men globally. It occurs when cells within the prostate gland grow rapidly and abnormally in comparison to normal cells. As is the case with many diseases, early detection is vital. Picking it up early increases survival rates, improves patient outcomes, and helps the patient's family manage the disease. The problem is, however, that accurate detection of the disease has been, and continues to be, a challenge.

There are a few main types of diagnostic techniques that medical professionals use. For example, when doctors suspect a patient has prostate cancer, they will conduct a 'prostate specific antigen', or 'PSA' test. This is a test that measures relative PSA levels – a chemical made by both healthy and cancerous prostate cells – in the blood. However, PSA test results can be quite unreliable. In fact, even those with normal PSA levels have been later found to have prostate cancer.

Another diagnostic tool is prostate biopsy. A biopsy removes small pieces of tissue from different parts of the prostate for examination under a microscope. The method used specifically for prostate cancer diagnosis is known as 'two-dimensional transrectal ultrasound', or 'TRUS', guided biopsy. In this technique, ultrasound imagery is used to guide sampling. However, TRUS guided biopsy also has limitations. It can be misdirected, and thus prone to sampling errors. In other words, the samples taken for biopsy are not representative of the cancer's severity – or they can even miss the cancer altogether.

So, in summary, there are currently no tests available with sufficient accuracy to screen men for early signs of prostate cancer. Therefore, scientists have been working tirelessly to develop better tests. One such scientist is Dr Baowei Fei, from the University of Texas (UT) at Dallas and UT Southwestern Medical Center, USA. His goal is to enhance the effectiveness of the TRUS guided biopsy technique by incorporating sensitive 'positron emission tomography' (PET) imagery.

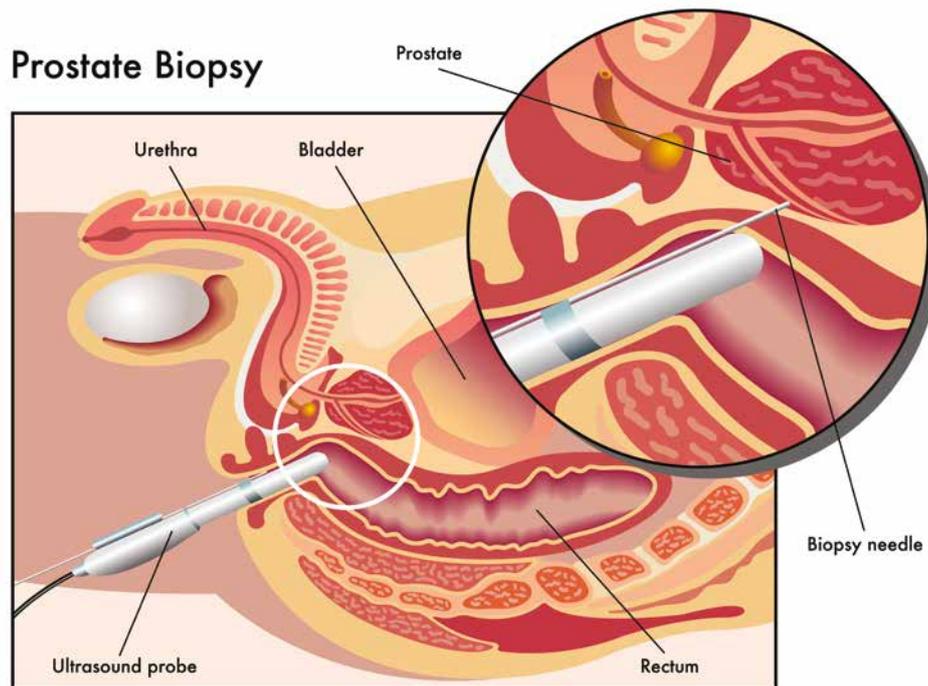


This multimodal approach produces detailed images of the prostate, and highlights areas of potential cancerous growth. With these images at their disposal, physicians can target biopsies to affected areas. This, in turn, produces more representative samples, and increases the likelihood of a correct cancer diagnosis.

Establishing the Merits of PET/TRUS Guided Biopsy

In research published in 2016, Dr Fei and his colleagues reviewed many of the current techniques for prostate cancer detection. They noted that

Prostate Biopsy



PET-based techniques can indeed provide a lot of information about the biochemical behaviour of a cancer. They also highlighted that it could be used in combination with ultrasound to guide biopsy sampling to areas of concern. 'Molecular image-directed, 3D ultrasound-guided biopsy represents a new trend for the diagnosis of prostate cancer and for monitoring of prostate cancer,' they concluded.

To consolidate this, in 2017, Dr Fei and a colleague conducted a review of the various applications of PET imaging-directed biopsy. They focused their review on cancers in a variety of areas of the body, such as the brain, bones, breasts, abdomen, pelvis, neck and vital organs – as well as glands such as the prostate. From that they concluded, 'PET-directed biopsy has an increasing role in the diagnosis and staging of various diseases.' Why? The guidance provided by molecular imagery, they noted, has great potential to increase the detection rate and improve diagnostic accuracy.

PET Molecular Imaging with New Radiotracer

Having proven that PET is effective for detecting disease, and especially cancer, Dr Fei wanted to hone a PET technique for the study of prostate cancer. For this purpose, Dr Fei and his colleagues needed to find a suitable radiotracer. In a medical context, a radiotracer is a compound that emits radiation from within the body of a patient. After adding a radiotracer to a patient's blood stream, for example, doctors get a map of metabolic activities and patterns. This gives them an insight into the tissue under examination at the molecular level. They can also add these compounds to tumours, glands or organs to survey the metabolism within them.

Dr Fei and his team selected a radiotracer that stood out above others – anti-1-amino-3-18F-fluorocyclobutane-1-carboxylic acid, or 18F fluciclovine (shortened to fluciclovine). This compound had already demonstrated its effectiveness in creating detailed PET imagery of tumour activity, so it was a natural choice for further research. Furthermore,

fluciclovine can isolate target areas as it is taken up more readily by cancerous tissue than by normal tissue.

To understand this process better though, Dr Fei and his colleagues examined the specific uptake behaviour of fluciclovine in the prostate. To do this, they introduced fluciclovine to two different sets of lesions – those that were malignant (cancerous) and others that were benign (not harmful). After appropriate uptake time, 3D imaging techniques were used to map the uptake of fluciclovine, and thus determine uptake effectiveness in the two different lesion types. The team confirmed what they had suspected – fluciclovine does indeed accumulate more readily in areas of cancerous growth and is an excellent radiotracer for differentiated imaging techniques involving cancer in the prostate.

How Fluciclovine Helps Doctors

In real terms, they now had a sure-fire way of differentiating between, and producing clear images of cancer-affected areas using fluciclovine. The subsequent biopsy that doctors take, therefore, can be guided to the exact



site of the tumour. This addresses the sampling errors common to other techniques, and therefore decreases the likelihood of a cancerous growth being missed.

More targeted biopsies also provide insight into the cancer's *aggressiveness*. Suppose a biopsy is taken from an area of minor cancerous growth, while an area of significant or aggressive growth is missed. The biopsy would still confirm that cancer is present. But it would also suggest that the cancer is only minor in nature. If the area of significant growth had been sampled, on the other hand, physicians would have a completely different picture of the disease. This has implications for the subsequent management of the disease, and thus, patient outcomes. So, Dr Fei's PET/TRUS technique is not just about detecting whether or not cancer is present, but rather, getting a full picture of its progression.

Having selected a robust and powerful technique, the question was – could PET be incorporated with TRUS to produce better imagery of the prostate, and guide biopsy sampling to areas of potential cancerous growth, in a real-world setting? Dr Fei and his team set out to investigate this question by way of a clinical trial.

PET/TRUS Guided Biopsy Proves to Be Effective

The purpose of the clinical trial was to see if using a PET scan and transrectal ultrasound (TRUS) guided biopsy together would detect prostate cancer more accurately than the standard 2D approach, which uses TRUS only to guide the biopsy.

In the trial, which Dr Fei and his team conducted in 2015–2017, the 21 participants were first injected with a solution containing the radiotracer fluciclovine. The patients then underwent abdominal and pelvic scans using PET. Next, an ultrasound probe, of about 2.5 centimetres in diameter, was inserted into the rectum of each patient. Using special apparatus, a 3D ultrasound image was then acquired from each patient's prostate.

However, when the ultrasound image was processed and *combined* with the original PET scans, Dr Fei and his colleagues could produce incredibly detailed 3D images of the prostate. And, most importantly, areas of suspected cancerous growth were clearer than ever. In fact, based on these composite images, the researchers could categorise suspicious regions as being 3 (equivocal), 4 (medium) or 5 (high), with regard to their potential to be cancerous. The team then guided the biopsy needle to these suspicious areas. They then processed these samples histologically for pathological examination.

The research team identified a total of 50 suspicious lesions with fluciclovine PET for the 21 patients involved in the study. The likelihood of a positive result using the TRUS guided biopsies that followed increased when the 'suspicious level' of the PET identified lesions increased (based on the team's categorisation system discussed above). In other words, cancerous growths, especially those that had been identified as more significant, were more readily detected when PET targeting was used in conjunction with traditional TRUS guided biopsy.

In summary, their method for targeted biopsy detected cancerous growth in 47.6% of patients, as opposed to 28.6% where typical biopsy methods were used. This increase in cancer detection rates was also achieved using fewer samples. This too is a significant result as their technique may reduce the time needed to treat patients and limit damage done to healthy tissue. Not only that, this study was the first-in-human trial that used PET imaging to direct 3D ultrasound-guided biopsy of the prostate. All round, the research was a great success.

Improving Outcomes for Patients with Prostate Cancer

Many different diagnostic tools are used to detect prostate cancer, such as PSA tests and standard TRUS guided biopsy. However, each one has limitations and many cancers are missed, or their severity is grossly underestimated. As a result, scientists and physicians are working to improve current diagnostic techniques. Dr Fei has been investigating the merits of PET, combined with the traditional TRUS method, as a more targeted method for prostate biopsy. His team's technique utilises an effective PET radiotracer, namely, fluciclovine. Other radiotracers, such as ⁶⁸Ga-PSMA, can also be used by this innovative technology.

Dr Fei's technique essentially combines high-sensitivity PET imagery with real-time information from ultrasound for improved cancer detection. A recent clinical trial, conducted by Dr Fei and colleagues, has demonstrated that this composite PET/TRUS guided biopsy method is more effective in terms of retrieving a representative sample, and making a correct diagnosis for prostate cancer, than the currently used TRUS-only technique.

As was noted at the outset, prostate cancer affects millions of people and has devastating effects on sufferers and their families. Of course, a complete cure for the disease is extremely sought after. In the meantime, however, improved diagnostics and early detection can improve patient treatment, and thus survival rates. By combining PET with the traditional TRUS guided biopsy method, Dr Fei and his team are working to improve prostate cancer detection, thus increasing the chances of a correct diagnosis.



Meet the researcher

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Dr Baowei Fei is Cecil H. and Ida Green Chair in Systems Biology Science, Full Professor of Bioengineering at the University of Texas (UT) at Dallas, and Professor of Radiology at UT Southwestern Medical Center. Before he was recruited to Dallas, Dr Fei was Associate Professor with tenure in the Department of Radiology and Imaging Sciences at Emory University, where he was Director of the Precision Imaging – Quantitative, Molecular & Image-Guided Technologies Program and Director of the Quantitative Bioimaging Laboratory. He was also a faculty member in the Department of Mathematics & Computer Science at Emory. Dr Fei was a Georgia Cancer Coalition Distinguished Scholar, served as a faculty member, and mentored PhD students in the Joint Department of Biomedical Engineering at Emory University and Georgia Institute of Technology. He received his PhD from Case Western Reserve University, Ohio, USA. Dr Fei's research interests include biomedical imaging, image-guided intervention, medical instrumentation, quantitative imaging, cancer treatment, hyperspectral imaging, image processing and analysis, artificial intelligence, machine learning and augmented reality. Dr Fei is a Fellow of the American Institute for Medical and Biological Engineering and a Fellow of the International Society for Optics and Photonics (SPIE). In recent times, Dr Fei has been researching the merits of PET/ultrasound guided biopsy as a means of effectively detecting prostate cancer – even taking the technique to clinical trials.

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FUNDING

National Institutes of Health (NIH)

FURTHER READING

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UT Southwestern
Medical Center

IMPROVING CANCER TREATMENT WITH NANOMEDICINE

Cancer is one of the most common causes of mortality worldwide and diagnosis rates are continually increasing. An estimated one in three women and one in two men will be diagnosed with a form of cancer at some point throughout our lives. For many cancer types, chemotherapy and radiotherapy are the chosen treatment methods, but their success rates are surprisingly limited, and both can cause serious side-effects. **Dr Afsaneh Lavasanifar** and her research group at the University of Alberta have set out to develop drug-delivery systems to improve the effectiveness of cancer treatment and reduce side-effects. Their research involves the targeted delivery of drug-loaded nanoparticles directly to tumour tissues.

The Need for Better Cancer Treatment

With the number of cancer diagnoses on the rise, successful treatment is becoming increasingly essential. Whilst chemotherapy and radiotherapy are frequently used to treat cancer, they can be ineffective in many cases and are extremely harmful to healthy tissues, resulting in a variety of serious side-effects.

Chemotherapy involves administering multiple drugs into a patient's bloodstream to destroy cancer cells. While such drugs have significant toxic effects in cancer cells, they are poorly specific for cancer and can also attack healthy tissue. Rather than exposing the patient's entire body to these anti-cancer drugs, delivering them directly to tumour tissues can significantly improve treatment outcomes and reduce side-effects.

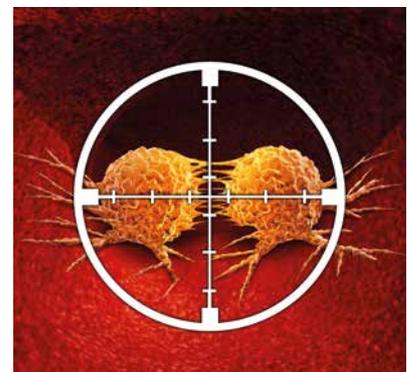
Likewise, radiotherapy involves a patient being exposed to large doses of radiation. While it can be effective

in destroying tumour cells, it can also have a negative impact on healthy tissue. The use of supplementary drugs delivered specifically to tumours during radiotherapy can improve treatment efficacy and allows the radiotherapist to use smaller doses of radiation.

Dr Afsaneh Lavasanifar, of the University of Alberta in Canada, has focused her research on the development of nanoparticles for drug delivery that can provide safer and more efficient treatment for those diagnosed with cancer. 'As a pharmacist by training, I have witnessed the adverse effects of medications in patients, first-hand,' says Dr Lavasanifar. 'In some cases, such as with anti-cancer chemotherapeutics, these side-effects are even more detrimental to the patient than the disease, itself, and significantly diminish the patient's quality of life.'

Therapeutic Nanocarriers

Nanomedicine, a fast-evolving area of research, involves the use of therapeutic



nanoparticles, and aims to improve on traditional drug administration techniques. Dr Lavasanifar and her team develop nanoparticles called 'nanocarriers' that can carry anti-cancer drugs to tumours to support cancer treatment, with the aim of increasing the specificity of such treatments for cancer cells. 'We are trying to make drugs in general and anti-cancer drugs in particular work better and have fewer side effects by redirecting them from healthy organs and cells to diseased tissues,' Dr Lavasanifar explains.

'The use of nanomedicine for new anti-cancer agents can prove to be a viable approach in bringing more new drugs with improved activity and reduced side-effects to clinical use.'



Nanocarriers are very small particles that can encapsulate other molecules, such as anti-cancer drugs, and transport them throughout the body. The use of nanocarriers for delivering drugs can sometimes be essential, such as when a drug is too delicate or insoluble to persist in the bloodstream on its own. Nanocarriers also make it easier to direct drugs to specific organs or tissues.

Dr Lavasanifar and her colleagues utilise 'micelles' as nanocarriers to encapsulate anti-cancer drugs. Micelles are tiny molecules no larger than 200 nm, which have a hydrophobic (water-repelling) core and a hydrophilic (water-attracting) shell. Their core can host different compounds and their shell allows them to be transported throughout the body without being detected by the immune system.

Dr Lavasanifar and her team chose these micelles because of their ability to encapsulate drugs that are insoluble in water and therefore cannot be administered into the bloodstream on their own. They are also safe for human administration as they are both biocompatible and biodegradable and can be excreted through the kidneys after they are no longer needed in the body.

Importantly, micelles also allow for passive tumour targeting, whereby they will preferentially accumulate in tumour tissues because of the leaky nature of tumour blood vessels. The small size of the micelles allows them to pass through small holes in these blood vessels, and they then accumulate in tumours, in a process known as the enhanced permeability and retention effect. As healthy tissues contain non-leaky blood vessels, the micelles do not tend to accumulate in such tissues.

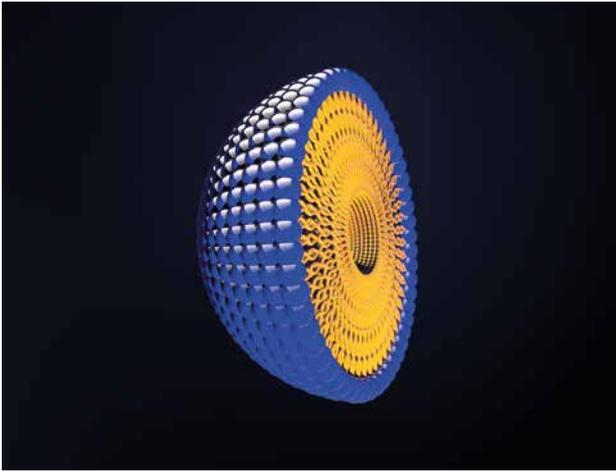
In 2006, Dr Lavasanifar and her team developed new micellar carriers and showed that they are more effective nanocarriers for the transportation of a variety of drug molecules. These newly developed nanocarriers have the potential to be modified to increase their clinical usefulness. These improvements include increased stability of the micelles, so that they can persist for longer in the body, while allowing more drug to accumulate in the target tumour. This project provided the catalyst for further research by the team, utilising these micelle nanocarriers for the delivery of specific anti-cancer compounds.

Active Targeting and Tracing

Dr Lavasanifar and her colleagues have also attached molecules to the surfaces of micelles that further facilitate their accumulation in tumours. In one recent study, the team attached a cancer-targeting molecule to two different types of micelles. This protein molecule can bind to other proteins that tend to be highly concentrated on the surfaces of breast cancer cells, thereby helping the micelle deliver its contents to the cancer cell.

Although this technique is highly advanced, the team found that the stability of the micelles had a greater impact on increasing accumulation in tumour tissue in a rat model, through 'passive tumour targeting', compared to attaching cancer-targeting molecules to the micelles.

The researchers confirmed the exceptional targeting ability of their micelles for tumours by tracking their location as they moved through the bodies of mice. The team was able to do this by incorporating dye molecules or contrast agents into their micelles, allowing them to be detected using imaging techniques.



This ability to trace nanocarriers after they are administered into the body can allow researchers to monitor their distribution and assess their usefulness in cancer treatments, while also ensuring their safety.

Overcoming Multidrug Resistance

Multidrug resistance (MDR) occurs when a tumour stops responding to treatment and can occur at any stage during a course of chemotherapy. It is thought to happen as a result of tumours eliminating or deactivating chemotherapy drugs, thereby protecting cancer cells from destruction.

Preventing MDR would greatly improve the chances of a given cancer treatment being successful. However, molecules that can inhibit the mechanisms tumours use to eliminate chemotherapy drugs lack specificity for cancer cells and can cause side-effects in healthy tissues, or make healthy cells sensitive to the effect of chemotherapy drugs. Because of this, such 'MDR inhibitors' have failed to achieve clinical approval to date.

A nanocarrier delivery system capable of achieving targeted delivery of these inhibitors would greatly enhance the treatment of MDR cancers. Such a nanocarrier would need to overcome the current limitations of MDR inhibitors, such as their poor stability, low cellular uptake, and rapid clearance from the bloodstream.

As part of their research into micelle nanocarriers, Dr Lavasanifar and her group have successfully shown that a chemotherapy drug and an MDR inhibitor can be encapsulated together within their micelles, for co-delivery to a tumour. In addition to relying on passive targeting, molecules attached to the surfaces of the micelles that bind to cancer cells ensure greater accumulation at the tumour site.

Inhibiting DNA Repair Systems

Cancer cells are often extremely good at repairing the damage caused by chemotherapy and radiotherapy, and contain

molecules that recognise and repair DNA breakages, negating the effects of many cancer treatments. Inhibiting these DNA-repair molecules from operating in tumour tissue improves the cancer's sensitivity to therapy. Likewise, it is also essential that these inhibitors accumulate in tumour tissue only, to allow healthy cells to continue the essential repair of damaged DNA.

After their success in delivering drugs to MDR cancer cells, Dr Lavasanifar and her colleagues used their micelle nanocarriers to encapsulate and deliver DNA-repair inhibitors to improve the sensitivity of colorectal cancers to treatment. Again, they improved the selectivity of these micelle nanocarriers by attaching molecules to their surfaces that specifically bind to molecules present on colorectal cancer cells. Furthermore, these micelles were no larger than 100 nm, allowing for substantial uptake and accumulation in tumour tissue. The group successfully demonstrated the targeted delivery of these micelle nanocarriers and the release of their therapeutic payload in colorectal cancers in mice.

Hydrogels for Drug Delivery

Dr Lavasanifar and her collaborators have also developed a 'hydrogel' formulation (called PolyGel™) from the same safe building blocks as their micelles. Drugs can be loaded into this substance, and it can then be applied to the skin or injected into tissues, where it can release a variety of drugs gradually.

PolyGel is a liquid at room temperature and forms a gel at body temperature. This formulation provides high stability and may be useful for a wide range of therapeutics. Dr Lavasanifar and her team have tested the hydrogel in animal models for the delivery of drugs to the surface of the eye and topical treatments for skin cancer treatment.

Future Directions

Overall Dr Lavasanifar's research has provided essential contributions to the field of nanomedicine. Specifically, this body of work has involved improving cancer treatments through the development of traceable micelle-based delivery systems that show excellent tumour-targeting ability.

'The use of nanomedicine for new anti-cancer agents can prove to be a viable approach in bringing more new drugs with improved activity and reduced side-effects to clinical use,' says Dr Lavasanifar. Towards this aim, her team is currently carrying out research to improve lung cancer treatment using micelles to prevent DNA repair in tumour cells. 'We are expediting the advancement of this new form of anti-cancer therapy in preclinical research.' The clinical use of these nanocarriers will undoubtedly have an overwhelmingly positive impact on the prognosis and quality of life for many patients in the future.



Meet the researcher

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Dr Afsaneh Lavasanifar gained her PhD from the University of Alberta in 2001, where she is now a Professor in the Faculty of Pharmacy and Pharmaceutical Sciences with a joint appointment in the Department of Chemical and Material Engineering. Her research encompasses the development of drug delivery systems to enhance therapeutics, with a specific focus on nanomedicine to improve cancer treatment. In addition to her academic research, Dr Lavasanifar holds numerous patents and is also the Scientific Chief Officer and Vice President of a spinoff company called 'Meros Polymers', which is founded on the technology developed by her lab. She is also the Associate Editor of *Molecular Pharmaceutics*, and a member of the editorial board for *Materials Sciences and Applications*. Dr Lavasanifar has received many awards and honors during her career, including the TEC Edmonton Innovation Makes Sense Award in 2013 and 2016, the Sanofi-Aventis/AFPC New Investigator Award in 2009 and the GSK CSPA Early Career Award in 2007 in recognition of her outstanding research in pharmacy.

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FUNDING

Natural Science and Engineering Council of Canada (NSERC)
Canadian Institute of Health Research (CIHR)
Canadian Foundation for Innovation (CFI)
Alberta Innovates Health Solutions (AIHS)
Alberta Cancer Foundation (ACF)

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WALKING AGAINST THE CURRENT

A research team at the University of Reading is helping people with paraplegia to stand, using electrical stimulation and high-tech exercise platforms to prevent long-term decline in bone and muscle.

Spinal cord injuries are far more common than you might think. Worldwide, somewhere between 250,000 and 500,000 people acquire a spinal cord injury every year. A car crash, a fall, or even an act of violence – all of these things can bring about an instant and massive change in someone's life.

Spinal cord injury affects people in more ways than just removing the ability to walk. The lack of activity causes the legs to lose strength, while both bones and muscles reduce in density. The act of standing and walking requires the legs to support the entire body weight and thus places a significant amount of pressure and loading on leg bones. Once this loading is gone, the body reacts by thinning out the unused bones – which in turn leads to a much higher chance of fractures. This effect is also seen in astronauts, where the long periods of weightlessness cause a similar lack of loading and thus bone density and muscle loss.

This is no surprise to those working in the field, such as Professor William Holderbaum and his research team at the University of Reading. 'People with paraplegia (those who have complete paralysis below the chest) often have weakened lower limb bones due to the total loss of leg movement,' says Professor Holderbaum. 'This leads to a reduced quality of life. The increased risk of fracture while performing daily activities such as transferring from and

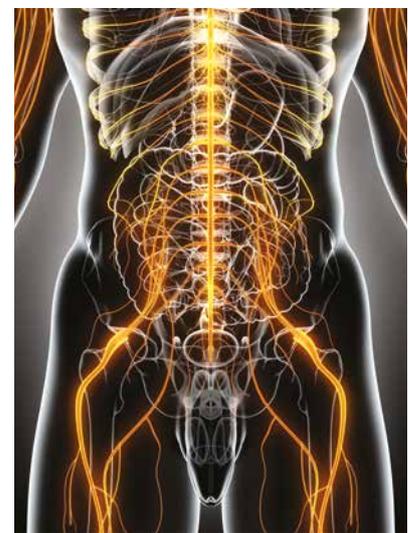
to the wheelchair may result in lengthy hospital stays. Additionally, such bone fractures significantly increase health risks and impact life span.'

The team of researchers is developing a therapy that will minimise this bone density loss, immensely improving the quality of life for those with paraplegia. As of yet there are no widely accepted ways to prevent or reverse this loss of bone density; pharmaceutical approaches do exist but tend to have significant side-effects. However, it is possible to slow density loss by simulating the typical forces caused by walking in a healthy subject. There are several ways to provide these forces, but one of the most effective is for the individual to stand up and shift their weight around.

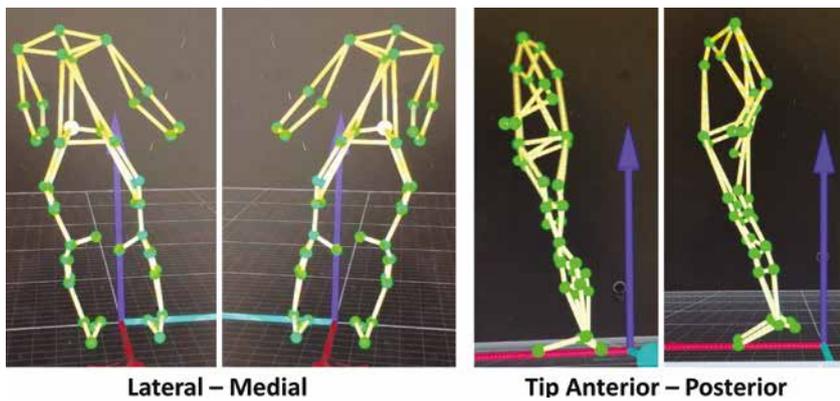
Standing Tall

It seems unlikely for someone with paraplegia to stand, yet technology has been available for many years to allow this. Known as 'functional electrical stimulation', or FES, the process uses electrical stimulation to induce muscle contraction.

In a typical muscle, nerve signals trigger the activation of an electrical impulse within the muscle filaments – this causes contraction of the filaments and thus contraction of the entire muscle. In FES, electrode pads are placed over the muscle to be activated and transmit a



low-energy electrical pulse. This pulse activates nearby nerve cells, which then transmit signals that activate the associated muscles. FES works in both healthy people and in those with spinal cord injuries – the injury does not take away the required nerve and muscle cells but merely removes the person's ability to voluntarily control them.



Lateral – Medial

Tip Anterior – Posterior



For a person with paraplegia, the FES system allows the main leg muscles to become activated, which has the effect of locking the legs in the extended position. Once this is done, the person can lean their upper body backwards to bring their centre of mass behind their back – in essentially an inverted ‘C’ shape. This creates a stable balanced posture that allows a person with paraplegia to stand upright, controlling their balance with upper-body movements.

There are some downsides to this technique, however. Electrified muscles do not rest and will begin to suffer fatigue, meaning that they will eventually fail to hold the locked-leg position required for standing. Many different approaches have been trialled to reduce muscle fatigue, ranging from changing the format of the electrical signals, shifting postures and activating specific muscles in different orders.

Framing the Solution

It is at this point that the Professor Holderbaum and his research team enter the picture. Their goal is to improve the currently available treatment of patients with paraplegia by more effectively slowing bone density loss. To do this, they have created one of the most advanced FES exercise platforms currently in use.

The platform is equipped with a number of sensors that measure the forces applied by the user. A motion capture system, similar to those used in the film industry, can record and reconstruct the current body position of the user. Using this data, a computer calculates which muscles to activate and when – a purpose-built FES device created by the team can activate up to 16 muscles at once to help users hold their balance and perform exercises.

A skiing video game demonstrates the current body posture and exercise output. This not only keeps users of the system entertained during the program but also provides instant feedback to ensure that the correct exercise posture is achieved. By co-ordinating FES and voluntary movement, the system provides exercise and leg loading while preventing the muscles from becoming too quickly fatigued. This entire process works with people who have paraplegia – it is essentially an automated standing and exercise device.

This system certainly sounds impressive, but the real question is whether it improves patient outcomes. To determine this, the team performed a study with the help of participants who had suffered a spinal cord injury. It was divided into two phases, termed leg conditioning and intervention. The leg conditioning phase consisted of a three-month training program involving daily use of the FES system designed to build leg muscle strength. This stage is vital for long term success – muscles begin to lose mass after only six weeks following a spinal cord injury, so it is imperative that prior strength is rebuilt before performing any standing exercises.

In the following intervention phase, the participants of the study were allowed to stand within the exercise platform, where they performed a number of load-bearing exercises as part of a skiing game. To ensure that the participants were ready for the process, the researchers first tested that they could undergo FES for one hour without showing significant signs of muscle fatigue and that they were able to balance by moving their upper body.

The participants came to the laboratory twice a week for six months to perform an hour of exercise. While in the exercise frame, the system used surface electrodes to stimulate between eight and 12 muscles in the lower limbs. This spread of muscle activation was performed so as to provide a wider loading of the bone and thus a more consistent degree of bone improvement



throughout. The research team designed the exercise program to focus on side-to-side and front-to-back movements – these motions are ideal for providing compression forces along the bone while avoiding shear forces across the bone, thereby minimising the chances of causing damage.

At the same time, the team used force sensors and motion capture systems to record the movement and forces being experienced by the participants. The researchers also took x-ray scans of the participants' legs, both before and after the intervention phase. They used this information to assess bone density in the affected areas and thus the effectiveness of the treatment.

'We found that our system shows an improvement of bone in certain areas, unlike previous systems which only decelerated the rate of bone loss,' states team member Dr Monica Armegol. 'We saw a small increase in bone density, even in those participants that were in the period of rapid bone loss. Although outcomes in bone density vary depending on the time since injury, the obtained results are really positive and encouraging for the spinal cord injury community.'

The information obtained from the intervention phase measurements was then used to adjust the parameters of a biomechanical model developed to simulate the characteristics of the participants. The ultimate goal of the model is to understand the distribution of internal forces in the bones and joints (e.g., ankles, knees, and hips) of the participants, especially as they perform various movements in the exercise frame. This is important for determining which stances lead to the best results in terms of bone development – for example, shifting the main force against the ground forwards on a foot increases pressure at the ankle by up to 60%.

It is well-established that there is a relationship between the force that bones are subjected to and the corresponding development of that bone. What is not well-understood is just how those factors interact – in particular the exact amount of force, and the frequency in which this has to occur for bone formation. The research team's goal is to more fully understand these interactions. Their hope is that the combination of biomechanical models and bone imaging will better link motion and bone response and thus the overall impact on bone health.

The Pace of the Future

So, where does Professor Holderbaum and his team want to go from here? There are many different goals and much work remaining. From a research point of view, the team is interested in studying more complex movements, and obtaining additional data to help them better predict when and where bone formation will occur. At the same time, the group is also interested in expanding the availability of the system, whether it be examining the role that these exercise-games can play in rehabilitation, or developing a home-based standing frame for wider accessibility.

This is just the first step on the long road to assisted walking for people with paraplegia – but if the work of the group is anything to go by, it will one day be a road well-travelled.



Meet the researchers

Dr Ioannis Dimitrios Zoulias
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Dr Ioannis Zoulias works with signal processing and control for safe FES-assisted standing of people with paraplegia. His research focuses on the clinical applications of human machine interactions. Dr Zoulias recently received funding from the Physiological Society to organise a symposium on transferring Brain-Machine interface technology into the clinic. He is a keen promoter of science outreach, and has a great track record in taking part in science public engagement events (for example, RI - Christmas Lectures (BBC) and Big Bang Science Fair).

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Professor William Holderbaum is a Professor in Mathematics and Engineering at the University of Reading, UK. Prior to this, he was a research assistant at the University of Glasgow in Scotland, UK. He was then appointed Lecturer at the University of Reading in October 2001, senior-lecturer in 2010 and Professor in 2014. He is also currently a Professor at the Manchester Metropolitan University and a Lecturer in Mathematics at the Open University. He has received government and charity funds to support his research projects in Functional Electrical Stimulation (FES) control and Robotics, the latest of which is the development of a FES system for bone health maintenance in spinal cord injury patients, funded by EPSRC.

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Dr Monica Armengol is interested in studying the biomechanics of different pathologies such as spinal cord injury and osteoarthritis. Her research focuses on the development of diagnostic tools and the design of better rehabilitation therapies. Dr Armengol is also very interested in transferring technology out of the lab and putting it into the hands of people. She has been awarded prizes for entrepreneurship and has taken part in many outreach events to encourage young women to pursue careers in STEM.

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FUNDING

EPSRC Project



JOINTS, VENTRICLES AND HISTORICAL BUILDINGS: A DIVERSE CAREER WITH STRUCTURAL MECHANICS

Engineering mechanics can provide medical researchers with invaluable insights into the diverse mechanisms contained within the human body, and the conditions that arise when they go wrong. Over a career spanning four decades, **Dr Nigel Shrive** at the University of Calgary has offered significant contributions to this field. His research is now helping to improve the lives of many millions of people who are currently suffering from mechanical failure within the body. Elsewhere, his work has also enabled countries to protect their priceless historical heritage.

A Sophisticated Machine

As one of the most sophisticated mechanical structures known to science, the human body exploits a diverse and complex array of systems to keep itself functioning in Earth's gravitational field. For most of us, a vast majority of these systems run so smoothly that we don't even consciously perceive them. However, with such uncertainty regarding the forces our bodies experience each day, and with so many processes playing out simultaneously, it is inevitable that some of them will occasionally go wrong, particularly as we age.

From joint pain to heart failure, anatomists have now spent centuries studying how the failure of certain biological mechanisms can give rise to our most unwanted ailments. Recently, the emergence of advanced new technology has provided researchers with unprecedented opportunities to study and correct these problems through surgery and artificial implants.

In each of these situations, however, there are numerous hurdles to

overcome before patients can return to their normal lives. In collaboration with medical colleagues, Dr Nigel Shrive at the University of Calgary explores innovative new ways to assess and treat various conditions, paying particular attention to tissues and joints, and the heart. The results of his basic-translational approach have led to several changes in clinical practice.

Failure in a Complex Mechanism

Our joints are among the most intricate mechanical structures in our bodies. To enable the ends of our bones to comfortably glide over each other, they are coated in smooth, rubber-like cartilage, surrounded by a lubricating synovial fluid, and tied to surrounding muscles through complex networks of tendons and ligaments. Yet as many people know all too well, there is much that can go wrong with the functioning of this complex apparatus. Clearly, a joint operates as an organ, an engineering system.

Among a variety of painful joint-related conditions is osteoarthritis, which commonly emerges in patients after an



injury to their joints. The disease is now known to result from a breakdown in bone and cartilage in the joints, which can cause symptoms including pain, stiffness, swelling, and a loss of motion.

Currently, osteoarthritis affects as many as one in six Canadians, and costs the nation's economy as much as 30 billion Canadian dollars each year. However, even with the latest advances in medical science, the current treatments on offer are severely limited in their ability to completely relieve patients of their



The robotic test system.

Advanced Robotics

Having gained a detailed knowledge of the biomechanical systems that joints use to function, and what happens when they fail, Dr Shrive and his colleagues used a robotic system to assess the mechanics of knee joints with pinpoint accuracy. Few previous studies had attempted to reproduce such artificial mechanics in the lab, since it was very difficult in the past to reproduce accurate motions in response to specific forces. However, through the latest advances in robotics, the researchers built a system that could move in a full range of 3D motions, and could rotate in any direction. Key to the accuracy of this system was a computational technique that closely tracked the motions of the robotic system, and adjusted them to become more realistic if they strayed off track. Through their tests, Dr Shrive's team reproduced the gait patterns of living sheep to within an accuracy of less than 1 millimetre, allowing them to compare the behaviours of individual tissues within their joints. The recent application of fibre optic technology in combination with the robotics has provided more unique information on joint functioning.

Through the success of this approach, the team's work could soon inform innovative new surgical techniques for reconstructing joints artificially. It may also allow researchers to identify new potential causes of osteoarthritis, which may lead to better treatments of the disease.

Pressure Overload in the Heart

Elsewhere in the body, the heart is another organ whose behaviour is dominated by complex mechanical processes, such as the interplay between the forces imparted by pumping muscle and the fluid dynamics of blood. In a study published in 2006, Dr Shrive and his cardiovascular colleagues examined the behaviour of the heart's 'septum', which separates the right ventricle (responsible for

life-altering symptoms, and repairing the damaged tissue is a mere hope. Alleviating this problem will require an in-depth knowledge of the functions of each of the tissues involved, how they respond to injury, and how they can best be repaired.

Assessing Joints After Injury

In a study published in 2004, Dr Shrive and his colleagues assessed the validity of a common idea regarding joint restoration: that in order to restore joint function, damaged tissues should be replaced with undamaged, 'normal' substitutes.

Through experiments, the multidisciplinary team showed that in many cases, 'less-than-normal' substitute tissues are better suited to the task. This is because each individual tissue in the joint has its own genetic and biological ability to adapt and remodel itself after an injury, in order to accommodate the changing biomechanical needs of the healing body. The team suggested that if these widely varied responses of different

joint components are not accounted for, any normal replacement tissues will ultimately come to face a far heavier share of the joint's workload, increasing the risk of another failure. In the joint 'organ system', each component has to function adequately for the system to retain optimal operation.

Through a further 2015 study, Dr Shrive and his colleagues examined how injury can result in changes to the properties of lubricating synovial fluid. Normally, the fluid contains a finely balanced mixture of protein molecules, but this composition can be profoundly altered by any disturbance resulting from injury. Through their experiments, the team found that after injury, the concentrations of one of its important proteins became substantially higher than normal, while another dropped to far lower levels. This resulted in changes to the fluid's lubrication properties, which accelerated the degradation of cartilage over time, increasing friction between bones.



A wall in the in-plane test rig.

pumping blood to the lungs to become oxygenated) from the left ventricle (which pumps oxygenated blood around the body).

At the time, researchers believed that this wall becomes deformed when the pulmonary artery is constricted. In turn, blood flow to the coronary artery becomes restricted, blocking the blood supply of the heart muscle itself. Due to the complexity of this process, it was very difficult for researchers to confirm this relationship through experiments.

The team solved the issue using a computer modelling technique, which breaks down complex systems into large sets of small, interacting parts – greatly simplifying their dynamics. Through these simulations, in combination with experiments, the researchers confirmed the relationship between septum deformation and pulmonary artery constriction for the first time. Their results also helped to explain why some patients with high blood pressure but no underlying heart conditions can experience angina-like chest pains.

New Assessments of Circulation

Through their latest research, the team has developed a general approach for understanding how blood flows, which

he believes provides a much-needed update to decades of misguided theories. Their ‘Reservoir-Wave Approach’ differentiates between two separate aspects of flowing blood: one related to the volume of the fluid; and the other, to the wave patterns it displays. Through experiments incorporating this approach, the team has provided potential new solutions to some phenomena that have long mystified medical researchers.

Among these insights is a potential answer to the exact function of the septum, and how changes to its behaviour can trigger angina in some circumstances. The Reservoir-Wave Approach could also help to explain why we don’t faint when we stand up quickly after lying down, even though the flow of blood to the brain is suddenly restricted. In addition, it could provide researchers with a far more complete toolset for exploring the nature of the complex interactions that take place between flowing blood, and the solid structure of the heart.

Protecting Historical Heritage

Alongside these important discoveries, Dr Shrive has also applied his expertise in a completely different area: protecting vulnerable historical buildings made

from brick and stone. On the Canadian government’s request, he helped to assess the Federal Parliament Buildings in Ottawa, which are seen by many as an irreplaceable piece of the nation’s heritage. At the time, authorities had decided that the buildings needed to be strengthened to withstand earthquakes so strong as to occur just once in around 2,500 years.

Through their analysis and testing, Dr Shrive and his colleagues determined that the structures are less flexible than more modern buildings. Unlike the latest materials, the brick and stone that make up the Parliament Buildings move in parallel to the motions of materials lower down – a behaviour that physicists call ‘shearing’.

This result provided authorities with invaluable information regarding where repairs needed to be made to preserve the buildings, while avoiding costly, unnecessary maintenance. The group’s predictions were then put to the ultimate test in 2010, when Ottawa was struck by a magnitude 5 earthquake. Just as they had calculated, the Parliament Buildings remained completely unscathed following the event.

Inspiring a New Generation

Throughout his 40-year career, Dr Shrive has provided researchers with a wealth of new insights into the mechanical forces at play in biological systems, and beyond. His discoveries ultimately culminated in the founding of the company Tenet Medical Engineering, which produced innovative equipment for improving the outcomes of orthopaedic surgery across Canada, sold equipment in over 50 countries worldwide, and has now been bought by a multinational.

Dr Shrive now hopes that his work will inspire a new generation of engineers, who will build upon his research to push the field of mechanical engineering in its many diverse forms.

Meet the researcher



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Dr Nigel Shrive completed his D.Phil. at Oxford University in 1974 where he invented 'The Oxford Knee', and has since worked at the University of Calgary for over 40 years. With research interests including the application of structural mechanics to masonry and heritage structures, and investigations of the mechanics of cells, tissues, joints, and the cardiovascular system, he is now a distinguished leader in the fields of both civil and biomechanical engineering. Elsewhere, Dr Shrive has promoted international collaboration between research teams in each of these disciplines, and has also focused on developing highly regarded mentorship schemes, creating one of the top graduate programs at the University of Calgary. He has been an elected Fellow of the Institution of Civil Engineers, UK, the Canadian Society for Civil Engineering, the Masonry Society, the Canadian Academy of Engineering, Engineers Canada and The Royal Society of Canada.

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FUNDING

Canadian Institutes of Health Research

The Arthritis Society

Natural Sciences and Engineering Research Council of Canada

Canadian Concrete Masonry Producers Association

The Canada Foundation for Innovation

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EVERYDAY CYBORGS: HOW OUGHT THE LAW TO DEAL WITH IMPLANTED MEDICAL DEVICES?

Attached and implanted technologies are now part of everyday life for many millions of people. Yet as the capabilities of these devices have advanced rapidly in recent years, lawmakers have struggled to keep pace. **Professor Muireann Quigley** at the University of Birmingham believes that it is now more critical than ever that the law catches up with the technological and social change wrought by attached and implanted medical devices, especially 'smart' ones. Through the Everyday Cyborgs 2.0 and DIY Diabetes projects, she and her colleagues hope to bring law, regulation, and policy regarding these technologies into the 21st century.

Attached and Implantable Technology

Not so long ago, the idea of advanced technologies being implanted into the human body seemed to be entirely confined to science fiction. However, as our ability to build devices that mimic the functions of our organs has improved, medical devices have become central to both the survival and wellbeing of many people who suffer from medical conditions. Moreover, these devices are becoming increasingly complex. Current generations of pacemakers, for example, run software, collect data, and transmit it remotely over Wi-Fi.

The emergence and growth of this technology now presents difficult yet urgent questions, including: Once a device has been implanted into a patient, do they have full ownership over the device and the software it depends on to function? How should the law respond to risks surrounding unauthorised third-party access or hacking of medical devices? Should

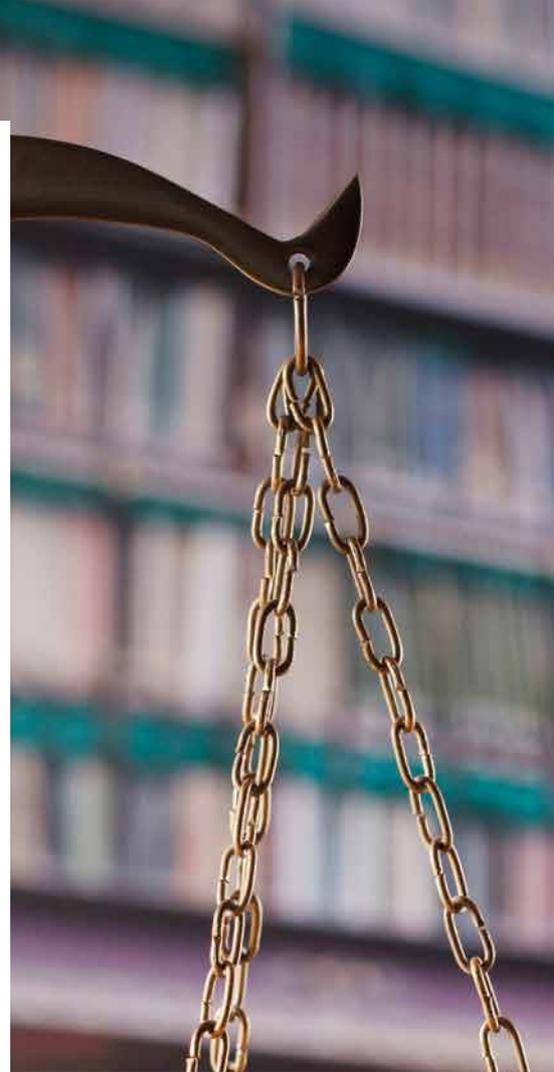
internal medical devices be viewed as part of the person, as mere objects, or as something else? Is damage to a person's implanted medical device a form of personal injury, or damage to property? Currently, the law lacks a coherent answer to these questions. As these devices become increasingly prevalent, answering these questions becomes ever more pressing.

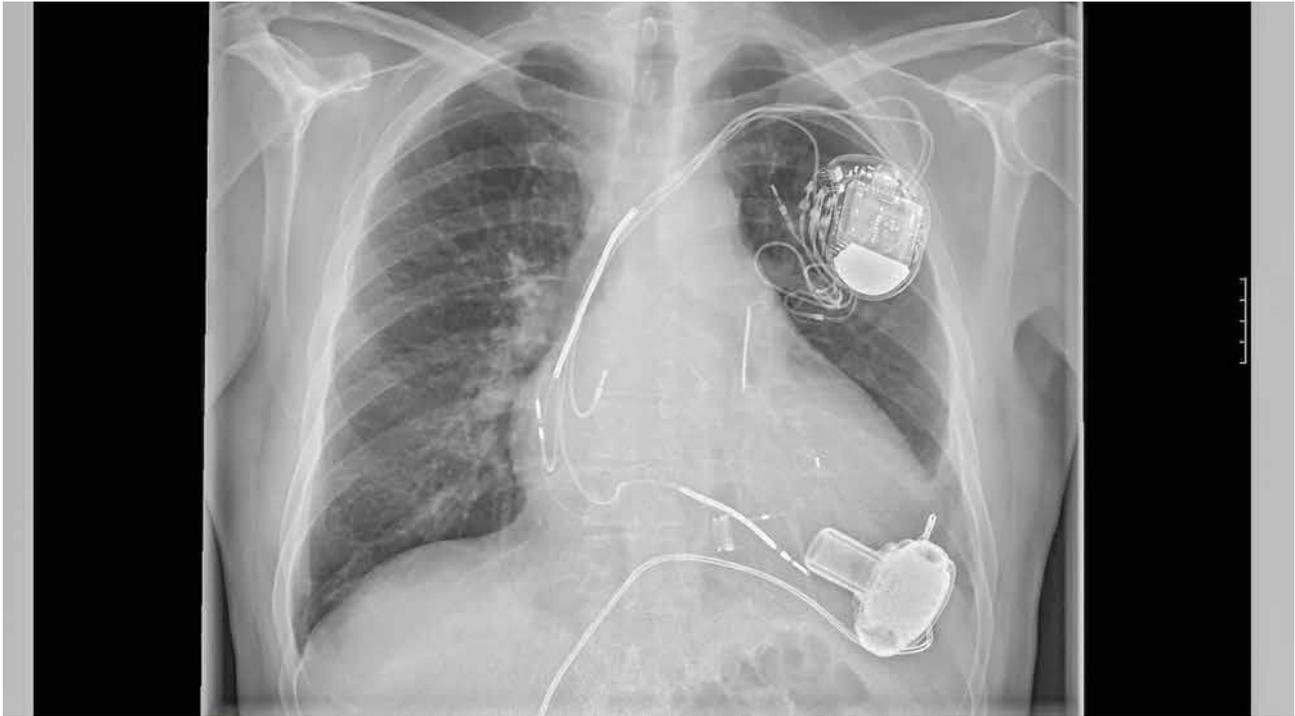
Legal Complexities

Professor Quigley's interest in these questions grew out of her longstanding work on bodies and separated biomaterials. In recent years, a growing number of cases have required lawmakers to reconsider how much say we can have over the use and treatment of materials originating from our bodies. This issue gained widespread attention when six men about to undergo chemotherapy, a process that can damage and even destroy fertility, deposited their sperm into a bank for safekeeping. Unfortunately, a malfunction in the storage system at the

fertility unit destroyed these samples. At the time, there was no clear answer as to whether these men were entitled to compensation for the loss of their sperm.

Eventually, the Court decided that the six had ownership of their sperm for the purposes of their claim and, as such, they had a right to compensation for the damage done. The case brought about a significant change in direction in the law regarding ownership over material that moves from the body to the outside world. Yet for Professor Quigley and her colleagues at the University of Birmingham, it also revealed how issues with the law not only related to materials being removed from the body,





but also to devices from the outside world being implanted into or attached to the body.

For devices that remain in the outside world, the law is reasonably clear. When we buy new devices such as smartphones or laptops, current laws state that you have ownership over their physical hardware, and that any damage to the device counts as damage to your personal property. However, the same is not true for the software run by the device. This means that by hacking into a device to alter its software, a user would be breaching the terms and conditions set out by the manufacturer, and could face a legal penalty or have devices ‘bricked’, rendering them useless.

Clearly, however, the situation becomes far more complex in the case of the software run by implanted medical devices. Whereas it may be permissible for manufacturers to impose penalties for unauthorised uses of consumer electronics, ‘bricking’ devices such as pacemakers, insulin pumps, or neuroprostheses could have devastating consequences for users. Ultimately, these issues stem from the fact that in its current state, the law says that something can either be a ‘person’

or a ‘thing’ – and cannot appropriately describe cases where external, non-living devices have been integrated into a body. Thus, there is much work to be done before legal practices can account for the realities of modern medical implants.

Introducing Everyday Cyborgs 2.0

Through their research, Professor Quigley and her colleagues aim to explore these problems in an interdisciplinary way, drawing on insights from Law, Socio-legal Studies, Philosophy, and Science and Technology Studies. The team ultimately hopes that their findings will inform law- and policymakers in how to best accommodate the increased blurring of boundaries between people’s bodies and the medical devices that keep them alive and healthy. Their efforts have culminated in the ‘Everyday Cyborgs 2.0’ project – a name that acknowledges attached and implanted smart medical devices are no longer confined to the realm of science fiction; they are an intrinsic and everyday part of people’s lives.

The team’s objectives can be summarised by three research questions. Firstly, what does the existence of everyday cyborgs (that is, persons with attached and implanted medical devices) reveal about the limits of current laws and policies regarding implanted medical devices? Secondly, what insights do we gain when these traditional legal, ethical and conceptual boundaries are broken down, and then reconstructed to account for hybridity between technology and the human body? And finally, how could policies and practices change after such a re-imagining?

A Roadmap for Research

These questions provide Professor Quigley’s team with an outline for a five-year research program. In the first two years of the Everyday Cyborgs 2.0 project, they will investigate where the law currently perceives the boundaries between people and medical devices to occur, and why they are there in the first place.

In the next two years, they will examine the pitfalls and opportunities that might arise when these boundaries are broken down. Finally, the team will develop a novel account of everyday cyborgs



in law. They hope that their new account will be empirically informed and practically useful, with solid conceptual and philosophical underpinnings.

Through these lines of inquiry, Professor Quigley hopes to resolve some of the unanswered questions outlined earlier. The insights gathered by Everyday Cyborgs 2.0 will come at a crucial time. As the speed of technological progress increases, our capacity to develop novel functionalities for our medical devices far outstrips legal and regulatory approval processes. In some areas, this regulatory lag has led to increasing numbers of patients with implanted medical devices developing their own Do-It-Yourself solutions, sidestepping official regulatory processes.

The Case of the Artificial Pancreas

One example is the development of Do-it-Yourself Artificial Pancreas Systems (DIY APS) by people with type 1 diabetes. In recent years, diabetes care has been revolutionised by the introduction of two pieces of technology: Continuous Glucose Monitors (CGMs), which monitor blood glucose levels, and insulin pumps, which deliver insulin through a cannula inserted under the skin. Based on readings from the CGM, a patient can manually program their pump to deliver a prescribed dose of insulin, to keep their blood glucose within safe levels.

Some patients, however, are dissatisfied with these devices for a number of reasons, including the level of insulin control offered and the amount of time they have to spend manually interacting with the devices. In response to this, a growing community of patients (sometimes called ‘loopers’) has emerged, who have taken it upon themselves to create their own DIY solutions.

Loopers construct their own DIY APS to better manage their diabetes. Following instructions available on the internet, they build open-source software that connects their insulin pump to their CGM via either a small computer or a smartphone. As the CGM tracks the patient’s glucose levels in real-time, the software calculates the optimal insulin dose required. This information is then transmitted to the patient’s insulin pump, which delivers the precisely calculated dose to the bloodstream automatically.

This system essentially allows the CGM and pump to talk to each other – creating a closed-loop system that makes continuous, automatic micro-adjustments to insulin levels. Users of these systems report benefits including reduced anxiety, less interrupted sleep, more time with blood glucose in the optimal range, and less time spent having to manage their diabetes (once the system is up and running). Together, these changes can significantly improve people’s quality of life.

The Confusing Legality of DIY APS

Despite these numerous reported advantages, some people are concerned about this technology from a legal standpoint. Firstly, DIY APS have not been through the process of regulatory approval, which commercially manufactured medical devices undergo to establish safety and efficacy. Secondly, the components of people’s DIY APS (the insulin pumps and CGMs) were not originally designed to work together in this way. Connecting them through the use of an open-source algorithm could constitute an unauthorised use of the devices – something that might violate the manufacturer’s user agreements, potentially voiding the warranties.

Thirdly, there is a particularly grey area regarding who should be held accountable if a looping system fails. Should it be the manufacturer of the component devices, the programmers who create the software, the healthcare service that prescribes the insulin pumps and CGMs, or the patient who uses these devices to build the DIY APS? Professor Quigley and her colleagues are just beginning to explore these issues through the DIY Diabetes project, which is running alongside Everyday Cyborgs 2.0.

#WeAreNotWaiting

Since ‘looping’ is a practice existing outside of today’s tightly regulated medical device industry, the legal implications are not clear. Many patients with diabetes are understandably unwilling to wait for the lengthy regulatory approval processes that could see approved artificial pancreas technologies become more widely available. This is exemplified by the looping community’s motto: #WeAreNotWaiting.

As part of the DIY Diabetes project, Professor Quigley and her team aim to take account of the views of the looping community and their clinicians, as well as device manufacturers, in order to address legal and ethical concerns regarding the use of such unregulated technology.

Preparing for the Future

Professor Quigley ultimately hopes that work on these projects will lead to much needed clarity with the law and regulation regarding attached and implanted technologies, bringing policies regarding smart medical devices into the modern age.

Meet the researchers



Professor Muireann Quigley

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Professor Quigley is Professor of Law, Medicine, and Technology at Birmingham Law School. Her interdisciplinary research focuses on three main areas: bodies and biomaterials, bodies and biotechnologies, and the use of the behavioural sciences in law and policy. In 2018, she brought together her findings on bodies and biomaterials in a major monograph, entitled: 'Self-ownership, Property Rights, & the Human Body: A Legal and Philosophical Analysis'. Professor Quigley is currently principal investigator on a 5-year Wellcome Trust funded project focusing on the legal and philosophical challenges that emerge when human bodies are joined with attached and implanted medical devices. She has also received a Quality-related Research (QR) grant from Research England and an Economic and Social Research Council Impact Acceleration Award for work on the regulation of DIY artificial pancreas systems.

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Dr Dickson specialises in the governance and regulation of legal subjects, and explores how the law impacts our ideas of personality and body autonomy. As part of the Everyday Cyborgs 2.0 project, she is studying the socio-legal aspects of medical devices, including the impact of the law on the diverse range of people involved in their use, including patients, healthcare professionals, manufacturers, and family members.

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Dr Joseph Roberts

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Dr Roberts currently focuses on the Everyday Cyborgs 2.0 project, where he explores the conceptual and normative questions posed by the joining of persons with attached and implanted medical devices. More broadly, Dr Roberts' research focuses on the notion of respect for persons and the limits of consent – specifically, whether or not people can truly consent to choices that will harm them.

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Dr Jessica Bell

University of Melbourne

Dr Bell works at the intersection of law, technology and health. Her research explores the legal and governance issues that arise in health and biomedical research. Dr Bell has expertise in the areas of health research governance, data protection and privacy and regulation of emerging technologies, and has been working on questions of liability regarding harm arising from DIY artificial pancreas systems.

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Dr Amber Dar

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Dr Dar has been conducting research on decision-making for and about children in relation to the use of DIY artificial pancreas systems. This involves analysing recent case law on 'innovative' or 'experimental' treatment and looking at how this should be interpreted and explained, with a particular focus on issues of parental responsibility and assessing the best interests of a child.

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Dr Laura Downey

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Dr Downey's research interests lie in the coproducing relationship between law, technology and society, and in further understanding law as both shaped by and shaping of the socio-technical environment. Her main focus is upon the interaction between law, regulation and emerging biotechnologies.

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Victoria Moore is a PhD student at the University of Manchester, whose doctoral research investigates legal and regulatory responses to patient safety incidents occurring during transitions of care. Her main research interests include the regulation of patient safety and medical professionalism. She has been working on issues concerning professional duties and clinician liability in relation to DIY artificial pancreas systems.

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Ms Amy Walker

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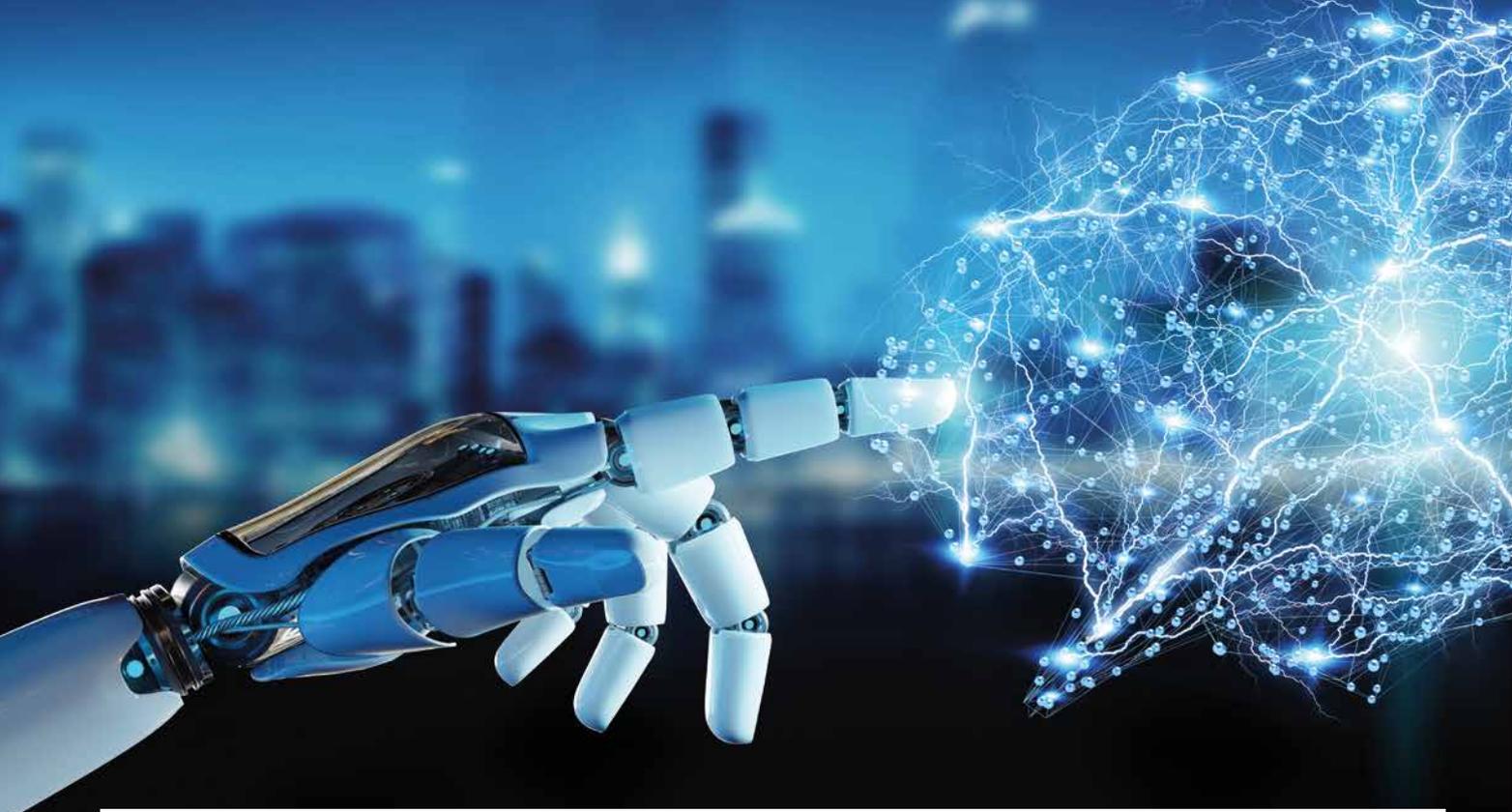
Amy Walker is a PhD student in Human Geography at the University of Birmingham. She has been reviewing the qualitative empirical research which has been undertaken with a range of actors related to DIY artificial pancreas technology.

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FUNDING

Wellcome Trust
Research England
Economic and Social Research Council

COMPUTER SCIENCE



TRANSFORMING SOCIETY THROUGH COMPUTING TECHNOLOGY

It's hard to think of something that has changed our lives more profoundly than computing. From healthcare to education, and from our jobs to our social lives, digital technology pervades almost every aspect of modern life.

In the COVID era, advances in computing have allowed for countless lives to be saved. Through their ability to rapidly process vast quantities of data, computer models are currently being used to monitor and predict the spread of the virus, speed up diagnosis, identify at-risk groups and rapidly screen thousands of potential drug treatments. Digital technology has also helped to curb viral transmission by enabling us to work, learn, shop and socialise without leaving our homes, which would have been impossible just two decades ago.

To celebrate these great achievements, this section of the edition features researchers who are spearheading the latest innovations in computing and data science.

As our last section focused on medical technology, the first article in this section introduces the work of Dr Juliana Bowles at the University of St Andrews, who uses advanced computational techniques to predict patients' responses to highly complex treatment guidelines. The team's software could enable patients with multiple chronic conditions to live more comfortable lives, with the peace of mind that their treatments are optimised and any harmful interactions are minimised.

Another way that computing technology is transforming healthcare is in the field of genomics. The ability to rapidly sequence a patient's DNA promises to make personalised, predictive, and preventative medicine a reality. In the battle against COVID-19, these advances also allow scientists to rapidly analyse the viral genome, enabling them to characterise individual viral isolates and track the spread of the disease.

However, not all scientists have access to the computing power required to process vast quantities of genomic data. To solve this problem, Dr Mark Miller and his colleagues at the San Diego Supercomputer Center developed the CIPRES Scientific Gateway. In our second article of this section, we discuss how this new gateway brings supercomputer-powered analysis to researchers across the globe.

Next, we focus on another crucial way that computing technology has helped to slow the spread of COVID-19: the ability to shop online and avoid busy shops. Here, we introduce Dr Hui Xiong and his colleagues at Rutgers University who have harnessed Big Data to better optimise online shopping for both cost efficiency and standard of service to customers.



Dr Timothy Young is another scientist who has found a new way to utilise Big Data for our benefit: streamlining the operations of manufacturing industries. Dr Young's numerous studies demonstrate beyond doubt that the vast amounts of data we continually collect can be immensely beneficial in ways that we may not initially expect.

From improving online shopping to predicting the spread of COVID-19, Big Data has proven to be invaluable in a variety of different areas. However, for many, the idea of Big Data is inseparable from the fear of a loss of privacy. Dr Florian Kerschbaum and his colleagues at the University of Waterloo aim to address this issue, through sophisticated new techniques that ensure complete anonymity for a company's users. If the team's methods become more widely adopted, they could reassure many people that their sensitive information is being handled properly.

Next, we showcase the research of Professor Manfred Broy and his colleagues at the Technical University of Munich, who are driving advances in the field of Software and Systems Engineering. Their work promises to make our software more reliable, secure and easy to use in our increasingly software-dependent world.

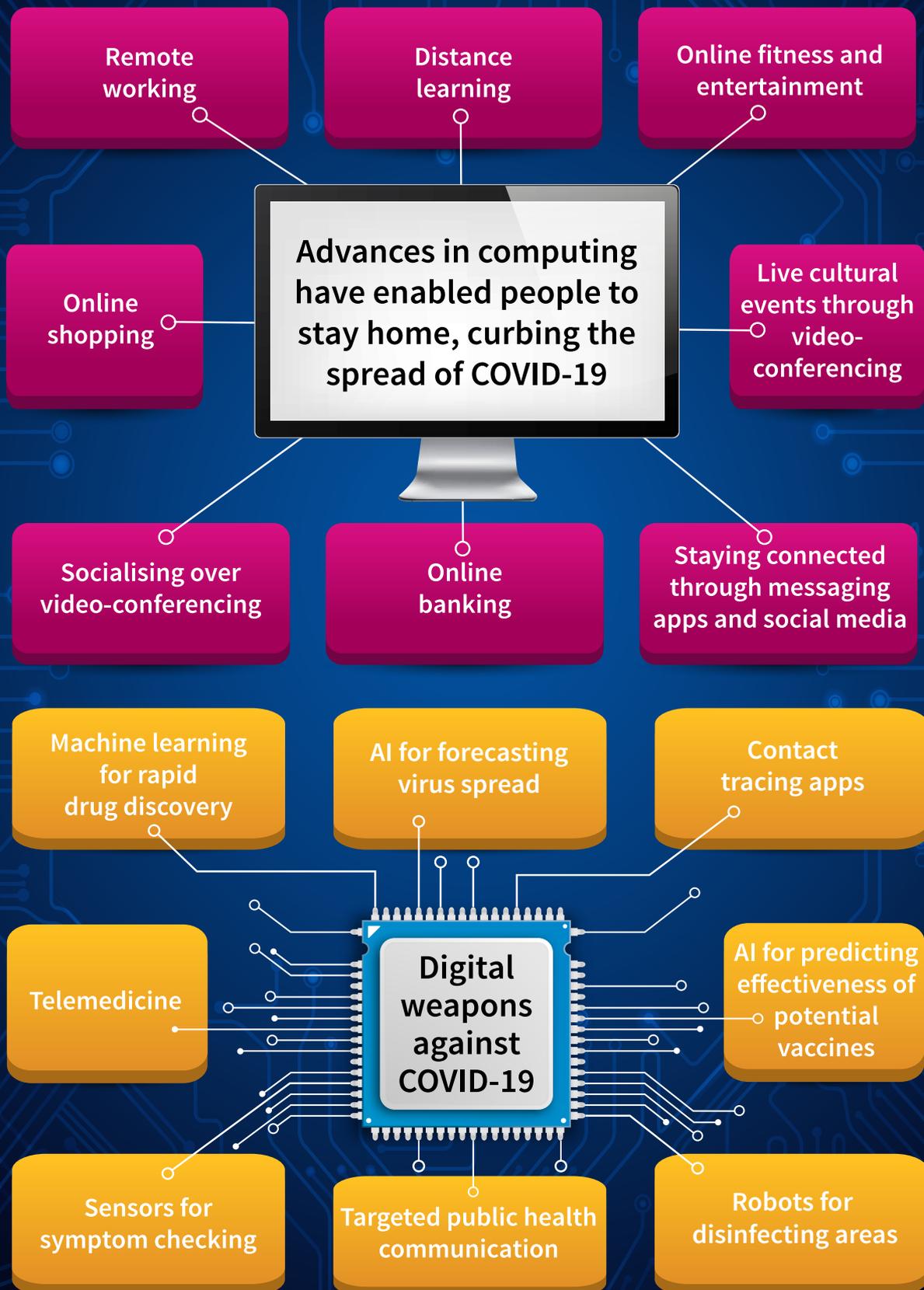
Also improving the reliability and safety of our electronic devices are Dr Rolf Drechsler and Dr Christoph Lüth of the German Research Centre for Artificial Intelligence, who we also meet in this section. This team has developed a new verification method called 'Self-Verification of Electronic Systems', or 'SELFIE', which aims to ensure the safety and efficiency of electronic systems within their real-world settings – saving time and money in the process.

The next part of this section plunges us into the world of machine learning, which is rapidly advancing the decision-making capabilities of today's computers. However, because this technology involves building complex models of the systems it will be applied to, many engineers and researchers find it inaccessible. To solve this problem, Dr Paul Robertson at Dynamic Object Language Labs has developed a language and toolchain that together are capable of building models themselves, using only robot sensor data. His team's approach could soon open up significant opportunities in the emerging field of artificial intelligence.

We then meet Dr Yan Yufik, of Virtual Structures Research Inc, who applies his understanding of the human brain to design machines that are not only able to learn, but can understand what they are learning. Rather than making predictions by extrapolating information from the past, Dr Yufik hopes that machines based on his theories will be able to derive predictions from actually understanding the past, paving the way for advanced artificial intelligence.

Our final article in this section explores the emerging technologies of Virtual Reality and Augmented Reality, both of which have surged since the beginning of the COVID-19 crisis. From enhancing online education to offering an effective way of experiencing cultural events, these technologies are playing increasingly prominent roles in helping people overcome the isolation brought by COVID-19. Here, we read how Dr William Hurst at Liverpool John Moores University is embracing Virtual and Augmented Reality to enhance education and business productivity, while providing insight into other ways that the technology may be used in the near future.

HOW COMPUTING INNOVATIONS AID THE FIGHT AGAINST COVID-19



COMPUTING CONFLICT-FREE TREATMENTS FOR MULTIPLE CHRONIC ILLNESSES

Modern treatments for patients with more than one chronic condition can be highly precarious, and in many cases, simultaneous treatments for different illnesses can be detrimental to each other and ultimately, the patient. **Dr Juliana Bowles** at the University of St Andrews believes that this pressing issue can be solved with the help of advanced computational techniques. Her team has explored the ability of such techniques to calculate reliable outcomes within models of complex systems. Their work promises to significantly enhance the ways in which treatments for chronic conditions could be delivered – improving safety and quality of life for patients.



Webs of Interactions

From natural ecosystems to social networks, the characteristics of many systems are driven by complex webs of interactions between different objects and components. To understand how they work, computer scientists can build behavioural models that predict the outcomes of manipulations to the system – all while obeying the laws of physics.

This approach has previously allowed researchers to virtually probe the

behaviours of a diverse range of systems. However, the technique faces one clear limitation: when systems become too large, and governed by many different aspects and variables, they can become far too complex for researchers to build accurate models of them.

To overcome the issue, computer scientists sometimes reflect on individual ‘scenarios of execution’ that are possible within complex systems. Instead of modelling the complete behaviour of a system, the concept

focuses on computing the outcomes of specific situations, brought about when systems are manipulated in specific ways. However, this approach has experienced pitfalls. Scenarios of execution can be carried out in a number of different ways, ultimately yielding many different, often conflicting outcomes. Consequently, the results gathered in the process remain inconclusive and unreliable.

Combining Computational Techniques

In their research, Dr Juliana Bowles and her team at the University of St Andrews have explored an improved approach which integrates a variety of so-called formal methods, including constraint solvers and theorem provers.

In particular, ‘satisfiability modulo theory’ (SMT) solvers allow the team to explore the use of arithmetic and add measures to find properties of interest. When formulating a problem as a series of logical constraints, an SMT solver tries to satisfy all the



constraints simultaneously, and if there are conflicting elements, it will identify them. A theorem prover can help to generate the constraints needed by the solver by expressing the problem in a simpler, more natural way. ‘In this context we use the theorem prover “Isabelle”,’ says Dr Bowles. ‘This has the added advantage that we can prove the correctness of the formulations directly within the theorem prover.’

Dr Bowles and Dr Marco Caminati, also at the University of St Andrews, developed an approach that explores the benefits of combining theorem provers and SMT solvers to generate outcomes in complex combinations of models. Their approach can ignore any present inconsistencies within the models, and only find scenarios of execution that are free from inconsistencies with each other.

Reaching Conflict-free Outcomes

By exploiting the advantages of combining Isabelle and SMT solvers, the team revealed that conflict-free outcomes of different scenarios of execution can be computed automatically. They also developed new ways to prove that their calculated results were correct and showed that their methods were more effective than when using solvers alone. To reduce complexity, Dr Bowles and Dr Caminati considered how some constraints of

behavioural models can be ranked over others if they are more significant, for instance if treatment of one disease, such as cancer, is prioritised above other comorbidities. They added further flexibility by allowing executions of different scenarios to start at different times.

Ultimately, the duo’s results paved the way for further studies regarding one of the most intricate systems known to science: the human body. In cases of illnesses enduring a lifetime, the body’s responses to highly complex treatment guidelines can be highly unpredictable. Dr Bowles and Dr Caminati realised that these inherent uncertainties have many similarities with the issues they had recently overcome.

‘Although software system specification and patient care guidelines seem different, inherently they have something in common,’ explains Dr Bowles. ‘In both cases we have procedures and executions of (partially) ordered sequences of actions, called “traces of execution” in computer science or “pathways” in clinical practice. In the case of computer-based systems, actions are carried out by users or computers, while in the case of care guidelines, actions are carried out by physicians, patients and carers.

In both cases, conflict may arise when individual executions and pathways are incompatible.’

Inconsistencies Between Treatments

The list of conditions that many people globally must endure for their entire lives is unfortunately long, including diabetes, heart and liver diseases, COPD and cancers. To ensure that patients suffering from these diseases have the highest possible lifespans and quality of life, clinicians have now developed treatment regimens incorporating factors including drugs, diet and lifestyle, which they recommend patients should strictly adhere to. So far, such efforts have reduced the suffering of many millions of people worldwide.

The evident problem with this approach is that some patients are likely to suffer from multiple, unrelated chronic conditions at the same time. Since patients dealing with these cases of ‘multimorbidity’ must be treated by multiple doctors, each specialised in just one of their conditions, they will inevitably receive multiple, often conflicting treatment guidelines at the same time.

Because these guidelines are so strict, it becomes highly likely that they will be detrimental to each other – forcing doctors to adapt their treatments to account for other conditions which they likely have little knowledge of. Ultimately, this means that the safety and wellbeing of patients already in challenging situations is at risk. According to Dr Bowles, this demands an urgent rethink in how computer science can further develop automated solutions aimed at improving the approach to treatment of multimorbidity.

Expanding Computational Capabilities

In a further 2019 study, Dr Bowles and her colleagues explored how their computational techniques could



be used to significantly streamline our current treatments of multimorbidity. 'We investigated automated methods of detection of conflicts in clinical pathways for multimorbidities and proposed solutions that resolve them,' she explains.

Building on results from Dr Bowles' previous study, the team presented their automated approach with clinical guidelines for specific treatments for chronic conditions. These instructions came in the form of treatment models. When translated into a form a computer could understand, the researchers' techniques were used to carry out scenarios of execution corresponding to a patient being treated with specific guidelines.

If two or more disease treatment models were fed into the framework, the SMT solver checked for any inconsistencies between them, indicating that one treatment was lowering the effectiveness of another. Subsequently, the correctness of the outcomes of the operation was checked by the automated theorem prover 'Isabelle', allowing either positive or negative scores to be assigned to each aspect of each clinical guideline. If any aspects were low or negatively scoring, the researchers could conclude that they were incompatible with other treatments and would need to be adapted.

Reaching the Best Compromise

For the first time, Dr Bowles' team had demonstrated a computational framework that could identify cases in which multiple clinical guidelines caused problems when carried out at the same time. 'We have shown how an automated framework combining efficient and formal verification techniques can be used to identify steps in different medical guidelines that cause problems if carried out together, and find the preferred alternative according to certain criteria, such as drug efficacy, prevalent disease, patient allergies,' she says.

Importantly, the software was able to consider factors including the interactions between two drugs, prescribed for different conditions; between foods and particular drugs; and contradictory health recommendations, including patterns of sleep and exercise. It also accounted for criteria unrelated to treatment, including patient allergies.

Through the scoring system established by the team's approach, doctors could be given clear guidelines as to the particular aspects of their treatments they need to adapt and aid them in finding a compromise treatment that would be more effective overall. With the success of this approach, Dr Bowles and her colleagues focussed on establishing greater flexibility in the computational framework, which will prove critical if the technique is to be integrated into practical treatments.

Establishing Guideline Flexibility

In reality, patients with multimorbidity will not only be concerned with the overall effectiveness of their multiple treatments; if their quality of life is to improve, a wide variety of other factors must also be considered. With this in mind, Dr Bowles and Dr Caminati have extended the capabilities of their technique further in their latest study. This time, they aimed to go beyond the consideration of medication effectiveness alone as their criteria for the best solution – checking for factors including the different stages of patients' conditions, and whether certain combinations of treatments were safe and comfortable for them.

If this is not the case, the software is now able to pick the best alternative from a group of potential medications. Furthermore, this list can be tailored to the personal preferences of the patient, including the avoidance of certain side-effects, while also accounting for the timing and dosage of the medication. If these conditions are not satisfied, the software can reverse its previous choices and go back to past decision points, enabling it to find solutions better suited to any pre-determined criteria.

Hope for Better Guidelines

The research of Dr Bowles, Dr Caminati and their colleagues is timely; multimorbidity is now a growing problem worldwide, with over half of people with chronic conditions in Scotland alone suffering from an additional comorbidity. Yet through the combination of SMT solvers with 'Isabelle', the team's software offers flexible solutions to the treatment requirements of a diverse range of patients. With this infrastructure in place, the researchers' techniques could now easily be adapted to account for other factors, including costs, the number of medications prescribed, and even biomarkers for targeted treatments, provided this information is known and available.

Through further research, Dr Bowles hopes to integrate the techniques into real clinical decision support systems, which will enable doctors to tailor their treatments both to the needs of their patients, and to the treatment guidelines of other conditions that they know less about. Her work now holds the promise to enable patients with incurable diseases to live more comfortable lives despite their conditions, with the peace of mind that the treatments they are receiving are optimised and that harmful side-effects and interactions are minimised.



Meet the researcher

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Dr Juliana Bowles was awarded her PhD at the Technical University Braunschweig, Germany, in 2000. After working as a postdoctoral researcher at the University of Edinburgh, she then took a lectureship position at the University of Birmingham in 2004. In 2007, Dr Bowles moved to the University of St Andrews in Scotland, where she is currently a Senior Lecturer in the School of Computer Science. Dr Bowles' research interests lie in the development of automated techniques for computer modelling, especially in healthcare. She is particularly dedicated to using computational methods to maximise safety and medication effectiveness for patients undergoing multiple treatments. She has presented her team's findings at several international conferences, in addition to events with the general public and GPs, which has generated considerable international interest. She also leads the EU Horizon 2020 research project SERUMS, which deals with the security and privacy of future-generation healthcare systems, putting patients at the centre of future healthcare provision, enhancing their personal care and maximising the quality of treatment they receive.

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FUNDING

EU Horizon 2020
HDR-UK
MRC
EPSRC

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CIPRES: A GATEWAY TO THE TREE OF LIFE

Modern genetics provides vast sets of information which can take weeks to assess. Developed by **Dr Mark Miller** and his colleagues at the San Diego Supercomputer Center, the CIPRES Scientific Gateway solves this problem, by bringing supercomputer-powered analysis to researchers across the globe.

Phylogenetics

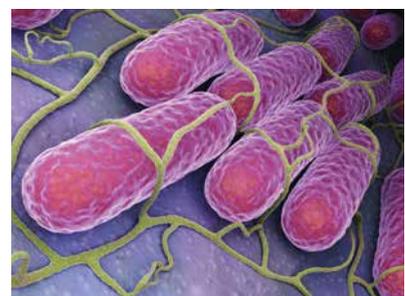
Cross the world and you will run into a dazzling array of life, from desert-dwelling mice to arctic birds, from sun-loving flowers to deep-sea microbes that will never see the light of day. Yet for all of these differences, every organism we find is related to every other one, somehow, even if we need to look back several billion years. But how do we know this? How do we decide whether two creatures are closely or distantly related? How is it even possible to know that *Tyrannosaurus Rex* is more closely related to a chicken than a Great White Shark is to a tuna fish? This is the science of phylogenetics – the study of evolution and how different species give rise to others.

The idea of a ‘tree of life’ is not a new one. Observant people have been placing animals and plants into groups and building relationships between them for hundreds of years. Yet until Darwin and his ground-breaking work in establishing the theory of evolution, no-one had thought that these groups may have developed from a common ancestor. Phylogenetics was built from this realisation – a scientific approach to plotting out the branches and leaves of the tree.

Early researchers built these plots from common features and appearance – a family of birds that looked like ducks and quacked like ducks were, in all probability, related to ducks. This works well in some situations but is often confused by convergent evolution – widely-separated organisms in a similar environment will often evolve towards a similar ‘optimal’ form. The classical example here is the eye, which has been independently developed by both vertebrates (mammals, birds, etc) and cephalopods (squid, octopus). Many more exist, and this makes things complicated for the scientist trying to determine how different species fit together.

This is where DNA sequencing enters the picture, which involves reading the ‘language’ encoded in our DNA. This technique can be used to record the entire sequence of an organism’s genetic makeup, or its ‘genome’. This genome can then be compared to that of other species to determine how similar they are to one another – a pair of sequences that are highly similar are likely to come from closely-related species, while those that are very different are likely from widely-separated ones.

Naturally, this is more complicated in the real world. Some DNA sequences are very important for all organisms and so remain similar across many





different species – genes involved in the production of RNA and proteins, for example, are almost universally conserved. Thus, scientists need to carefully choose the genes to be compared, and indeed a reliable phylogenetic study requires the analysis of many different genes. And therein lies the current problem.

Drowning in a Sea of DNA

Thanks to the many advances in DNA sequencing, it is now possible to rapidly and cheaply collect vast amounts of genetic data. It currently costs a patient between \$1000 and \$2000 USD to have their genome completely sequenced. Scientists focusing on smaller sections of DNA can have sequences determined for less than the cost of a coffee. ‘DNA sequencing techniques have become very cheap and very fast,’ notes Dr Mark Miller of the San Diego Supercomputer Center. ‘The phylogenetic field has been catapulted into a world where discovery is no longer limited by the amount of available data.’ But all of this data comes with a cost, as this flood of information needs to be *understood*.

Collection of sequence data is fast, simple, and cheap, yet actually analysing this data is a serious bottleneck for the scientific process. ‘As more DNA sequence data has become available, routine analyses that used to run in a day on laptop now require a week or a month,’ notes Dr Miller. ‘The alignment of this data, and analysing the differences are computationally hard. The amount of time required increases exponentially as the length of the DNA sequence and the number of species being examined increases.’

This is a problem for many researchers, who mostly work from standard desktop computers or laptops that lack the processing power to do multiple analyses in parallel. ‘Performance is impacted by this kind of analysis,’ says Dr Miller, ‘and usually only one such analysis can be run per computer.’ Pushing the calculations onto dedicated computer clusters is possible, but requires that the researcher actually has access to such a high-performance machine and that the right software is installed, updated and maintained.

CIPRES: The Power Plant of Phylogenetics

This is where CIPRES enters the picture. The CIPRES Scientific Gateway (derived from ‘**Cyber Infrastructure for Phylogenetic RESEARCH**’) was initially thought up as a response to these problems faced by the scientific community. Developed and improved by Dr Miller and his colleagues over the past decade, it has turned into a central hub for much research going on today. CIPRES provides a web-based access point to a number of up-to-date and efficient phylogenetic programs, all running on local supercomputers. Researchers simply need to register, upload their data, choose from a number of approaches, and then go and grab a cup of coffee. Preferably a coffee to go, as many of the analyses will be finished within minutes rather than the hours or weeks that a personal computer would require.

The CIPRES Scientific Gateway achieves this speed in two ways. First, it has access to an incredible amount of raw



computing power through a connection to the supercomputers of the National Science Foundation. Secondly, the CIPRES team installs applications (created by others in the field) that run typical phylogenetic analyses in parallel. In other words, rather than taking the data and performing the overall analysis one step at a time, the process is broken up into many different steps, which can be performed alongside each other. This is tricky from a programming point of view but is extremely effective at speeding up the overall process.

‘CIPRES allows users to upload their data, and can run as many as 50 analyses concurrently,’ says Dr Miller. ‘Most analyses also run 10–200 times faster on CIPRES, because we have up-to-date, optimised parallel codes installed on very large computer clusters funded by the US National Science Foundation.’

This essentially makes CIPRES a vital piece of supporting equipment for phylogenetic scientists. By providing access to an assortment of computing resources, the gateway accelerates the pace of research beyond what would otherwise be possible. ‘We provide a service that makes it possible to research, much like the waterworks supplies water that makes it possible to live in cities,’ explains Dr Miller. ‘Most of our users say things would be slower or be halted without the access we provide – what we do is to make research go faster.’

CIPRES has had a noticeable impact on the field of phylogenetics. Access to the gateway is free, allowing researchers from across the world to take advantage of the computing power despite any lack of funding. Indeed, the list of users ranges from NASA through to the Korean National Arboretum. Tens of thousands of researchers have used the gateway to date, with more than 5,500 publications arising through the support of CIPRES in the first nine years of operations. Many ground-breaking studies published in prestigious journals such as *Science* and *Nature* have only been possible due to the rapid analysis of genomic data available through the gateway.

Importantly for scientists, the nuts and bolts of maintaining, tuning, and updating the software are performed by experts at the CIPRES group. This means that scientists can focus on the ‘biological thinking’ parts of their research, while freeing them from the daily worries of patching software and maintaining computers. ‘CIPRES makes it easy for a biologist who is not computer-literate to access and use a highly sophisticated machine to ask important biological questions without months of training,’ says Dr Miller.

The Gateway of the Future

So where does Dr Miller and the CIPRES team intend to go from here? They have a number of plans for the future, many of which involve improvements to the user experience. They plan to develop simpler processes for restarting analyses in the middle of a run, as well as complete automation of the upload, input verification and analysis process. They have also just received a grant from the National Science Foundation to implement the rather niftily-named ‘cloudburst’ into their system. This allows the CIPRES gateway to use cloud computing power when the number of user requests overwhelms even the supercomputer power at their site.

Many other improvements are on the horizon, but Dr Miller is careful not to bring too many ideas onto the field at once. ‘We are very judicious with innovation,’ he comments, ‘we are constantly trying to improve our services – but we have to do so knowing that 10,000 users will be impacted by any changes we make.’

The CIPRES gateway has already shown its value, helping thousands of scientists achieve their work faster than they ever could alone. What will this new wave of improvements bring? Only time will tell – but it is likely to involve further ground-breaking scientific discoveries and ever-more satisfied researchers across the globe.



Meet the researcher

Dr Mark Miller

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Dr Mark Miller received a BS in Biology at Eckerd College in 1972 and PhD in Biochemistry from Purdue University in 1984. He joined the Department of Chemistry at the University of California as a researcher in 1986, where he studied enzyme structure-function relationships. In 2000, he moved across campus to the San Diego Supercomputer Center, where he is currently a Principal Investigator. He is responsible for developing the CIPRES Scientific Gateway, which allows researchers across the world to enjoy high-speed analysis of genomic data.

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FUNDING

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National Institutes of Health

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SDSC SAN DIEGO
SUPERCOMPUTER CENTER

HARNESSING BIG DATA TO IDENTIFY IDEAL LOCATIONS FOR WAREHOUSES AND BIKE SHARE STATIONS

With a sharp increase in the public use of online shopping in recent years, which has spiked further due to the COVID-19 pandemic, the importance of warehouse positioning to provide an optimal delivery service has become a significant area of focus for retailers. Similarly, bike sharing in major cities has also seen an astronomical rise in usage – prompting questions about how bike stations can be best positioned. Stations in optimised locations would require minimal interference to change the stock levels, while also ensuring the greatest accessibility to users. **Dr Xiong** and his colleagues at Rutgers University have been using the ubiquity of big data to better optimise these systems for both cost efficiency and standard of service to customers, testing their findings in real-world scenarios.



Warehouse Site Selection for E-Commerce

Being an extremely competitive market, e-commerce businesses must find slight advantages over competition in order to boost their profits. One of the biggest draws for customers who shop online is fast delivery – the convenience of ordering an item one day and having it delivered the next.

To make this a viable option, e-commerce companies have to be able to effectively tackle the so-called

‘connected capacitated warehouse location problem’. This, in its essence, aims to minimise the costs of shipping (supplier to warehouse), delivery (warehouse to customer) and the inter-warehouse transportation involved in keeping stock levels adequate. Optimal warehouse positioning is pivotal in making this happen.

A big first step in choosing warehouse locations is being able to predict how sales will be distributed geographically, depending on how effectively retail delivery can operate. However, most

available predictive models struggle to find patterns between different logistical factors and customer satisfaction, and so are strictly limited in their prediction accuracy and usability.

A New Model for Warehouse Locations

In a paper for the 2017 International Conference on Data Mining, Dr Xiong and his colleagues at Rutgers University provide a ‘data smart approach’ to the connected capacitated warehouse location problem. Firstly, the researchers address the problem of predicting customer demand. ‘When all other factors are equal – including retailer reputation score and product quality evaluation – customers are more willing to choose the retailers with fast shipping, fast delivery and high-quality logistics,’ Dr Xiong notes.

As such, his team has built their predictive model around three factors that are known to influence customer demand: the time taken for an item



to be shipped after an order is confirmed, the time between an order being shipped and arriving at a customer, and the prevalence of damaged items after being shipped. The model is then driven by an artificial neural network – a network inspired by the human brain that allows computers to learn patterns and identify relationships based on input data, and subsequently carry out a human-like decision-making process. For Dr Xiong's research, this means using real-world logistics data for the three influencing factors previously listed and then producing a prediction of customer demand.

In fact, during their study, Dr Xiong's team put their new model to the test, using data from almost 3.5 million transactions that took place in 2012 on a Chinese online shopping site called Xiaoye. Using other predictive algorithms for comparison, the researchers showed that their neural network model was significantly more accurate, with an error rate of 27.25% – compared to 28.99% achieved using the next-best model.

Interestingly, their analysis also showed that customers are more likely to opt for a delivery service with shorter shipping time but longer delivery time than the other way around. This indicates that the transport of goods from supplier to warehouse is of greater importance than that from the warehouse to customer, meaning that keeping warehouse stock levels consistent is paramount.

This finding is the main driver in the team's algorithm for choosing optimal warehouse locations. Their algorithm keeps computational costs about 40% lower than alternatives, and works on the principle of assigning customers to warehouse locations that minimise logistics costs. Ultimately, Dr Xiong and his colleagues showed that having a network of four connected warehouses is much more effective in managing stock levels and keeping shipping costs low than having one centralised warehouse – bolstering the argument for warehouse networks.

The Rise of Bike Share Systems

Another important application of the research carried out by Dr Xiong and his colleagues is bike sharing. Bike sharing systems are now prevalent in many major cities around the world, with



their usage in New York alone accounting for 17.58 million trips across 329 stations between the summers of 2013 and 2015. They appeal to both commuters and tourists alike, providing a healthy and cheap option for short distance journeys and filling in gaps where public transport is limited or unavailable. Just like the surge in online shopping, the use of bike sharing systems has also witnessed a significant rise during the COVID-19 pandemic, as they provide a far safer alternative to public transport.

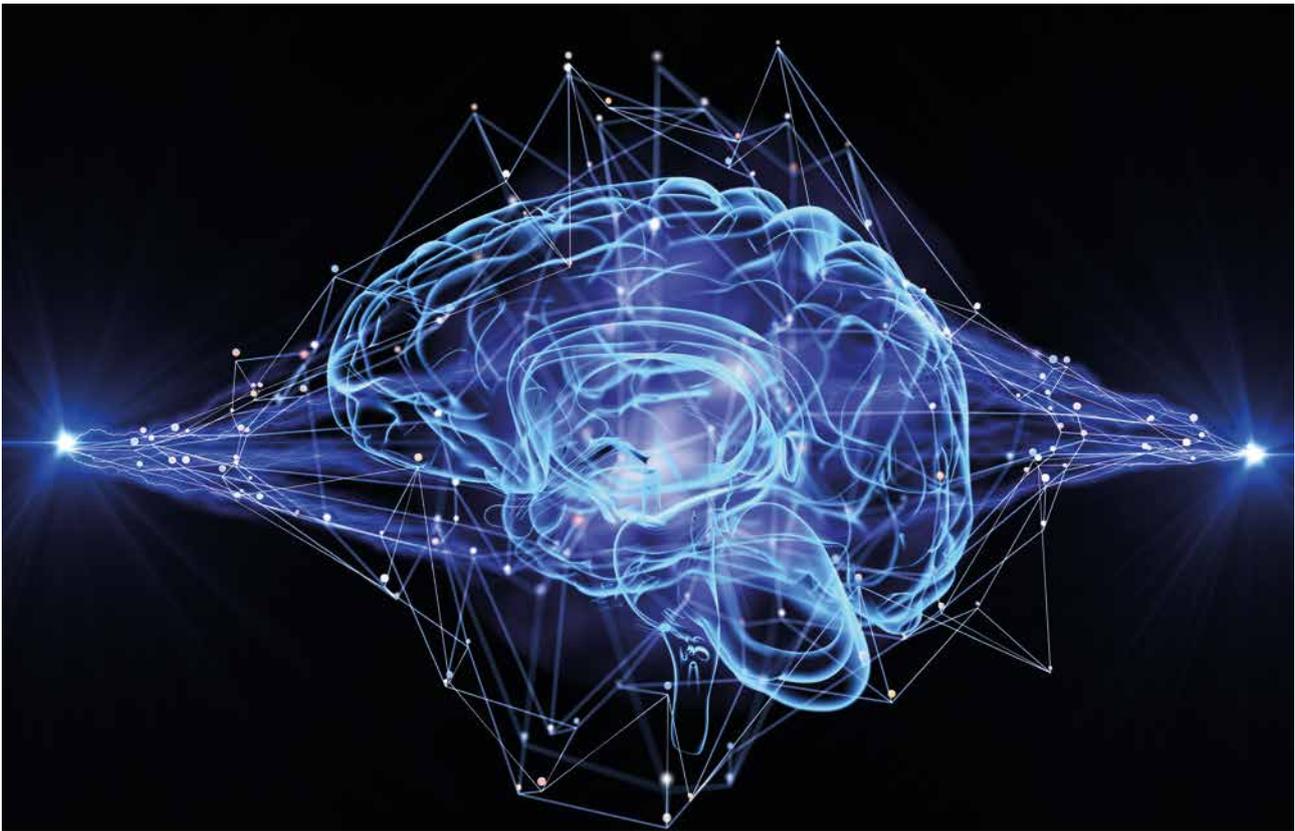
As a result of their increasing popularity, many cities such as New York are looking to expand their current system and implement more pickup and drop-off locations for the bikes. However, this comes with numerous challenges.

The new stations need to be effective in providing the public with access to bikes in locations that are prone to high demand, such as those between subway stations and corporate buildings for morning commuters. At the same time, the stations need to maintain an acceptable stock level – ideally never short of bikes and also never becoming overfilled. In other words, new stations should allow for a self-sustaining network where incoming bikes replace outgoing ones. If this is not the case, rebalancing operations must take place, which involves transporting bikes from one location to another – an additional expense for companies running the bike stations. This system should of course come hand in hand with the bikes being available at busy locations and covering popular journeys.

Taking this into consideration, bike share companies need to use a predictive model that can take into account a variety of influencing factors and guide the positioning of stations within cities. So far, the current models have only been able to use bike usage patterns and station demand data, whereas influencing factors of geographical bike demand have not been properly investigated.

Rebalancing Bike Share Systems

Using a similar artificial neural network model to that used for warehouse positioning, Dr Xiong's team has also produced



remarkable results in predicting customer demand for bike sharing systems, and keeping stock levels balanced at stations. This time, the data inputted into the artificial neural network included walking distances between bike stations, walking distances from bike stations to underground entrances, density of taxis in particular regions and points of interest in particular regions.

Applying the model to data from 256 of New York's CitiBike stations, the team showed that their neural network model had an accuracy of 85.2% in predicting bike demand, revealing 185 stations as being balanced and 71 as unbalanced. The level of accuracy achieved was a significant improvement over alternative models.

Showing further advancements in this area, Dr Xiong and his colleagues have played an integral role in solving the rebalancing problem – that is, minimising the costs in rebalancing bike stock – by implementing a new programming method.

As noted by Dr Xiong, 'Clustering can be used to reduce the complexity of the large-scale optimisation problem.' Clustering works by grouping certain bike stations together, and having the stock in these particular groups serviced by one vehicle. The stations are grouped based on functional zones – areas that have similar surrounding points of interest and are located relatively close-by to one another.

Certain functional zones will contain self-sustaining stations that don't need to have their bike stock rebalanced by non-users. Others will need vehicles to deliver or collect stock to maintain appropriate numbers of bikes. This method effectively changes a large-scale problem of great complexity with bike stock controlled by multiple vehicles, into simpler problems for individual areas with stock controlled by only one vehicle. Once this is achieved, the vehicle rebalancing route can be optimised to be significantly more efficient.

Using real-world bike trip data and weather data covering 328 bike stations in New York's CitiBike scheme, the new vehicle routing method – based on clustering – proved to be much more effective than the so-called Nearest Neighbour Insertion Algorithm – a routing method generally praised for being an effective solution to the problem. This is thought to be due to the small distances covered in the clustering scheme compared to the long-distance nature of the Nearest Neighbour Insertion Algorithm, which adds complexity and consequently cost to the problem.

Into the Future

Through their extensive research, Dr Xiong and his colleagues have demonstrated effective solutions to both the connected capacitated warehouse location problem and the bike share rebalancing problem. As the COVID-19 pandemic has caused an increased need for optimised bike sharing schemes and online shopping, the team's research comes at a pertinent time, and will likely lead to great advancements for bike hire and retail companies alike.



Meet the researcher

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Dr Hui Xiong graduated with a PhD in Computer Science in 2005 from the University of Minnesota – Twin Cities. A recipient of the IEEE Fellow award and the Ram Charan Management Practice award from Harvard Business Review, among many other individual accolades, Dr Xiong received two-year early tenure in 2009 and the RBS Dean’s Research Professorship in 2016 at Rutgers University. His research primarily focuses on the application of data analytics for developing efficient solutions for data intensive tasks. An esteemed publisher of numerous peer-reviewed and conference papers, Dr Xiong has also edited *Encyclopaedia of GIS*, a top 10 most popular computer science book written by Chinese Scholars as recognised by the major publisher Springer. In addition to his research, which garners national and international attention, Dr Xiong is heavily involved in mentoring PhD students, 16 of whom have graduated to date and the majority of whom have become tenure-track professors in renowned universities in the world.

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US National Science Foundation

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AI AND DATA MINING FOR SMART MANUFACTURING

Big data is now central to the operation of many online companies, but until now, the wealth of information it provides has remained largely untapped by manufacturers. **Dr Tim Young** at the University of Tennessee believes that through data science, this information could be used to significantly streamline the operations of many manufacturing industries. His work provides the widely varied parties involved in these processes with important new insights into how they should handle their data, ultimately helping them to improve the efficiency of their operations.



Getting the Most out of Big Data

Never before in human history have we had access to such a vast amount of data. With the advent of technologies including smartphones and advanced sensors, constant floods of information are now being collected for purposes ranging from better movie suggestions on Netflix, to improving the flow of road traffic.

However, Dr Tim Young at the University of Tennessee believes that the use of big data still has significant untapped potential in manufacturing industries. Thanks to decades of previous research, statistics and data science

have produced many sophisticated techniques for exploiting the huge amounts of data collected by these industries, each of which processes information in different ways.

Despite this progress, the widespread use of big data in manufacturing still faces significant challenges. Although the algorithms involved can be applied to many different situations, the sheer diversity of these tools makes it incredibly difficult for non-specialists to decide which approaches are best suited to particular tasks.

To overcome this issue, manufacturers must work together with data scientists to ensure that the statistical analysis they use to process information is actually useful. In his research, Dr Young applies his expertise to explore how these different algorithms can best be used to exploit data gathered throughout manufacturing processes involving biological materials.

A Dilemma in Wood Composite Manufacture

Wood composites, such as particleboard and structural engineered panels, are important materials in the construction and manufacturing industries. Although they have different strength properties relative to regular wood, they are far cheaper and lighter, making them more desirable for many purposes. To manufacture these panels, particles and fibres of pulverised wood are mixed with resin, formed into flat sheets, and are then often treated with other chemicals. This process is more complex than it sounds: for a high-quality final product, bonds between individual wood grains must be strong, and the panels must be reasonably resistant to rupturing when subjected to mechanical forces.



To ensure this level of quality, manufacturers need to use just the right proportions and properties of wood fibres, resin and chemical treatments, and add them to the mixture at just the right times. With so many possible combinations, it is extremely difficult for manufacturers to optimise their processes. In the face of this challenge, statistical analysis can come into play: by identifying algorithms that accurately model how the quality of the final product will be affected by individual aspects of the production process in real time, solutions for optimising processes can be found far more easily.

Improvements Through Statistical Analysis

Through a series of studies, Dr Young and his colleagues assessed the real-time performance of several different ‘kernel regression’ and ‘deep learning’ algorithms. Among the most widely used families of algorithms in data science, these models are statistical tools for estimating relationships between multiple strength and process variables. For their purposes, Dr Young’s team used real-time data gathered by sensors to make real-time predictions of the bond strength between wood fibres, and the points at which the panels would fail in modulus and tensile strengths in the final product.

The team validated the accuracy of these predictions, to identify which algorithms are more effective than the others. Through this work, one regression model consistently emerged as a possible candidate for having the best real-time predictive performance. This Bayesian algorithm, which is common in robotics, incorporates mathematical structures from ‘kernel tree methods’, whose multiple branches represent a hierarchy of variable interactions within the process, and whose leaves represent optimum end points for the variable being predicted. Applied to a manufacturing context, Dr Young’s team showed that this algorithm, if used in real-time settings, can prevent the manufacture of low strength panels, identify sources of variation in the process, and possibly lower the costs of expensive additives while using less energy.

Streamlining Transport Flows

Ensuring quality in final products is just one aspect of Dr Young’s research. Before useful consumer products can be

assembled, they must sometimes first be fabricated at separate facilities, and then transported to a central factory. For wood composites, important aspects of this part of the production process include procuring fibre, timely transportation over tens to hundreds of kilometres to a factory to avoid wood decay, and processing in a timely fashion to produce high-quality particles. This throws up several more important factors for manufacturers to consider, including wood age, mill locations and road delays – all of which can affect the overall production efficiency.

Using the huge amounts of data gathered by wood composite manufacturers in the southeastern US, Dr Young’s team again used statistical analyses to determine the regions in which material transport is currently the most streamlined. This time, they incorporated a different type of logistic regression model into their algorithms, which was better suited to identifying optimum locations for biomass-using facilities. Through their analyses, the researchers identified certain parts Alabama, Georgia, North Carolina and the Mississippi delta as particularly well-suited areas for large-scale material production and transport.

Quantifying Disruption from Natural Disasters

Even further down the chain of production, the growth of raw materials can be made far less certain through weather complications, with potential disruptions including heavy rains, strong winds, and ice storms. In more extreme circumstances, these events can damage the plantations needed to produce wood, although this is often far more likely to happen in some regions than others. Through statistical analysis of a national database, Dr Young and his colleagues identified particular regions where local governments have reported more frequent responses to natural disasters than others.

As they did this, the researchers accounted for the influence of ‘risk’ from natural disasters on aspects including the types and ages of the trees being grown, and social and environmental disruptions in local regions. Through these calculations, the team could categorise different regions by the extent to which composite wood manufacturing would be disrupted by extreme weather. Out of the 33 states they analysed, they



identified inland parts of Georgia, South Carolina and Texas with high tree growth potential and low risk – important in manufacturing for a secure fibre supply.

Controlling Material Quality

Another area explored by Dr Young and his colleagues involves the properties of processed biological materials themselves, which can be highly variable, depending on several further factors. The overall quality of a biobased material can strongly depend on the uniformity of three separate factors throughout the material: wood particle sizes, ash content and moisture content. Any variability in these three factors can significantly reduce the quality of the final product, thereby incurring losses for the manufacturer. Using statistical algorithms commonly used in quality control, Dr Young and his team quantified the severity of each of these impacts.

In their study, the team concluded that variability in the three factors could increase production costs by between \$10 and \$20 per tonne of final product – making it critical for manufacturers to ensure uniformity in particle size, ash contaminant and moisture content early on in the process.

To do this, Dr Young introduced a new technique in a further study, in which the chemical spectra signatures of materials are picked up by real-time infrared sensors before manufacturing begins. By subjecting these signatures to the same algorithms used in the previous study, any unwanted variation can be revealed in the early stages of the process, allowing manufacturers to adjust their mixtures before significant costs are incurred. If implemented into factories, Dr Young hopes that this technique could enable manufacturers to ensure higher quality in their final products.

Examining Economic Potential of Biofuels

Finally, Dr Young has applied his expertise to consider how statistical analyses could be used to aid the production of

biofuels. Through a survey spanning two decades, the US government has already gained important insights into the economic potential of these sustainable fuels. However, questions remain as to how their production is affected by biomass yields, logistical operations, and the integration of systems between plant growth and harvest. This highlights a critical need to understand the impact of a wide variety of factors, including soils, climates, plant growth and the economics of biofuel plantations.

Again, Dr Young's team has shown that with the appropriate algorithms, data on each of these factors can be accounted for in optimising the production of biofuels. For four different plant species, the team analysed each factor to determine the economic potential of biofuel plantations in specific regions of the US.

The improved insights gained through this study could now prove to be an important step forward in our understanding of the benefits and precautions involved in biofuel production. Importantly, it could also influence future efforts to sequester carbon into the ground, which could become a key aspect of future sustainable economies.

A Wealth of Opportunities

Through their thorough analysis of manufacturing processes centred around bio-based materials and biomass, Dr Young and his colleagues have clearly demonstrated the numerous benefits that big data can offer for all parties involved. His discoveries show that when the right algorithms are applied, factors ranging from weather patterns to road delays can be accounted for in economic models.

Thanks to this success, Dr Young's numerous studies demonstrate beyond doubt that the vast amounts of data we continually collect can be immensely beneficial in ways that we may not at first expect.



Meet the researcher

Dr Timothy Young
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Dr Tim Young completed his PhD in Statistics (Natural Resources) at the University of Tennessee (UT) in 2007. He now works in the Center for Renewable Carbon at UT, where he became a tenured professor in 2010. Dr Young's research interests currently include real-time data analytics for use in manufacturing processes involving biological materials, a web-based economic model for improving the sustainability of biomass production, and data science education programs geared towards manufacturing. He has received numerous awards for his research, including a fellowship in the International Academy of Wood Sciences in 2019 and 'Alumni of the Year' from the University of Wisconsin in 2018.

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FUNDING

Grants and contract funding exceeding \$18 million from a multitude of sources from the private sector including Arauco North America, Assured Bio Labs, Brown Forman Corp., Georgia-Pacific Corp., J.M. Huber Corp., to name a few. Government grants are primarily from US Department of Agriculture US Department of Energy, and US State Department.

TAKING THE STING OUT OF BIG DATA

To many people, the idea of Big Data is inseparable from the fear of a loss of privacy. Since many modern companies must collect vast amounts of personal information in order to operate effectively, this concern is now growing globally. **Dr Florian Kerschbaum** and his colleagues at the University of Waterloo aim to address the issues presented by this reality, through sophisticated new techniques that ensure all-encompassing privacy for a company's users. If the team's methods become more widely adopted, they could reassure many people that their sensitive information is being handled properly.



Data Flow

Many of the services we use in our everyday lives involve a flow of data from us, as users, to private companies, which typically store the information in their servers. Yet this flow is much more than a simple transaction: from the transfer of data through third parties, to the categorisation of the information it contains, the overall field of Big Data involves several distinct and important steps, before data can be effectively managed and manipulated by users.

Firstly, data is acquired as user information and is transferred to a server. Then it is prepared, as new data in the server is matched up with the user who provided it. At the management stage, server data is processed as it is subjected to operations by users; and through analysis and modelling, they can more easily access the information they need. Finally, use and inference involve categorising the data, making it easier for users to deal with. As a whole, this data pipeline runs so smoothly that we barely notice it. However, its operation still faces one particularly serious challenge.

Protection at Every Stage

In recent years, the issue of our right to privacy over the information that Big Data companies collect from us has gained widespread attention. It stems from the fact that much of this information is so personal and sensitive, that significant amounts of damage could be done if it fell into the wrong hands. Yet just as the data pipeline is intricately complex, the measures that would be required to ensure sufficient user privacy at each of the steps it involves are difficult to define.

In their research, Dr Florian Kerschbaum and his colleagues at the University of Waterloo have developed wide-ranging measures to combat this issue – each based around the concept that full user privacy is a fundamental requirement. In collaboration with SAP, a software company in Germany that relies on Big Data, and the Royal Bank of Canada, Canada's largest financial institution, the researchers have now applied their new techniques to several different situations, representing each stage of the data pipeline. As Dr Kerschbaum puts it, his work aims to 'take the sting' out of Big Data once and for all.



Acquisition

When companies collect information about their users, users can't necessarily trust the company to anonymise their data. To maintain privacy, therefore, the data must be transmitted in a distorted form, meaning that the company cannot read the value of a single user.

However, the company should be able to obtain aggregate data about a collection of its users. This can be achieved by a large distortion that cancels out over the aggregation, but if any user fails to transmit, the aggregate is unusable. Another way that this can be achieved is through a small distortion that diminishes over the aggregation, but many users are needed for an accurate aggregation.

Dr Kerschbaum and his team present a new computational technique based on statistics and cryptography, which can quickly and accurately gather private information through untrusted parties. These parties, which can be a few users or distributed servers, aggregate first and then apply a very small distortion. 'This involves collecting data from users with privacy and without a trusted collector,' Dr Kerschbaum summarises. 'Google and Apple collect user data with privacy, but their methods do not scale to lower than millions of users. We can do it for thousands of users.'

Preparation

Once data has been collected, another challenge arises: since multiple companies can possess information about single users, they often need to work together to identify matches in their records of individual people across multiple datasets. As they do this, two companies comparing records must use computer programs which can make these connections automatically, but this creates a significant privacy concern. If an individual has disclosed some information to one of the companies, but not the other, it would be a breach of their privacy for that data to be shared between both companies.

Again, there have been previous computational techniques that combat this issue, but they have typically come at the cost

of reducing the accuracy and time efficiency of the matches. Now, Dr Kerschbaum and his colleagues have developed a new approach that offers full security for all parties involved, while maintaining high performance. 'This involves linking data across parties without disclosing it – which is done very often, but without data protection,' he explains. 'We hope to be able to scale it with data protection, and I am now thinking of founding a start-up on this idea.'

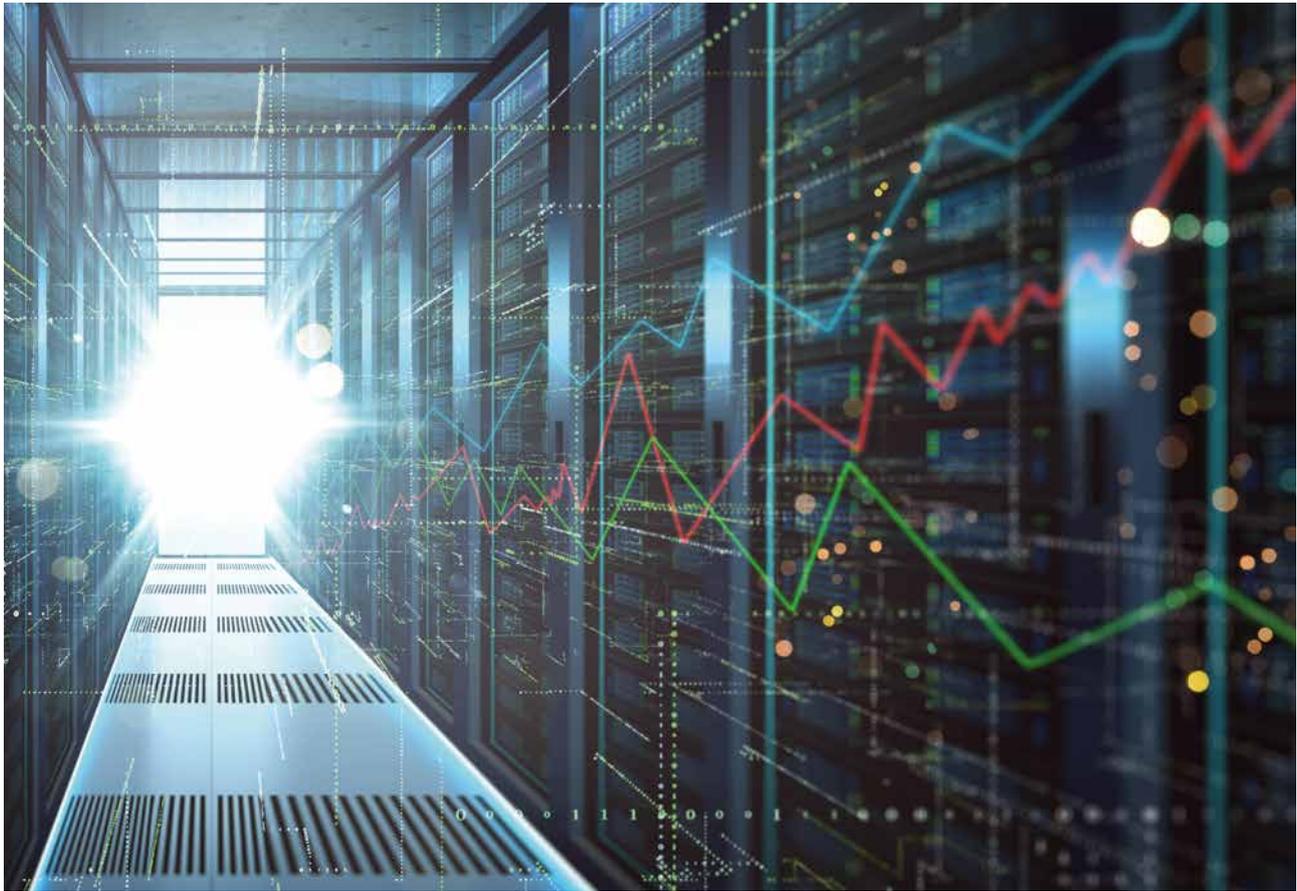
Management

When we use the services provided by a Big Data company, we are essentially commanding operations to be carried out on our own sensitive information while it is being held on their servers. However, as companies execute these operations for us, they must continually read and write new sensitive information, creating a further risk to user security. To alleviate this risk, companies must use databases that aren't able to 'see' the data they read and write. This is particularly important for cloud databases, in which users can store vast amounts of information on company servers in an encrypted form.

To achieve such a computationally demanding task, Dr Kerschbaum has developed an algorithm that is 'oblivious' to the data it operates on, which can account for realistic hardware and security capabilities of both users and companies. The structure of this algorithm makes it highly secure in various settings, while maintaining simplicity, operational efficiency, and high performance. 'Here, we focus on using secure hardware to process encrypted data in the cloud,' Dr Kerschbaum describes. 'This allows us to create a database that doesn't see what it is processing.'

Analysis and Modelling

Computers can exploit some useful techniques to help us analyse, organise, and retrieve our documents, which are key components of user-friendly interfaces. Sometimes, however, these same techniques can be used for more sinister purposes. There are many situations in which document writers might prefer to remain anonymous – from giving negative customer feedback, to criticising a restrictive government. Yet by



determining how frequently particular letter combinations are used in a document, and then checking these frequencies against previous reference texts, groups can often identify the authors of anonymous documents simply by the terms or phrases they use on a regular basis.

Dr Kerschbaum and his team have introduced an approach that artificially alters the terms used in original documents, altering their term frequencies, while retaining their meaning. This makes it far harder for hostile groups to use techniques to determine the authors of anonymous documents, without diminishing the accuracy of such otherwise useful identification tools. As Dr Kerschbaum summarises, 'this involves building a model of a textual database that protects private information, but also allows non-sensitive inferences, such as the identification of which news group a post belongs to.'

Use and Inference

When data has been gathered onto a server, it often needs to be categorised in order to make it easier to access and use. This can be done using tools named 'decision trees'. Based on the capabilities of artificial intelligence, these models are now used in applications ranging from spam filtering to healthcare. However, difficulties arise when servers use decision trees to classify user information, while maintaining their privacy. This requires the end results of decisions to be revealed to the user, while nothing is revealed to the server after the process has finished.

Currently, the existing techniques for doing this require many steps, making them computationally inefficient. Dr Kerschbaum's team has combated the issue by restructuring the decision tree so that it only shares the outcome of one branching point with the next point – enabling privacy to be maintained throughout the operation.

The team has now used the technique to categorise a large, real-world dataset – significantly reducing the computation time compared with previous approaches. 'The class of a data sample held at a client is inferred, using a decision tree held at a server,' Dr Kerschbaum explains. 'This is done without disclosing either the data sample to the server or the decision tree to the client using computation on encrypted data.'

Removing the Sting

Within the current technological landscape, it now seems increasingly inevitable that Big Data will play an ever-growing role in our lives going into the future. While many people are justifiably fearful over what this reality might entail, Dr Kerschbaum believes that his team's techniques could ensure that our personal information can never be compromised in such a world. By viewing privacy as a central requirement in every step of the data pipeline, the sting of Big Data could finally be removed, ensuring a more secure future for everyone.



Meet the researcher

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Dr Florian Kerschbaum completed his Doctorate in Computer Science at Karlsruhe Institute of Technology in 2010. He has worked as an Associate Professor at the at the University of Waterloo since 2017, has been Director of the Waterloo Cybersecurity and Privacy Institute since 2018 and was named the NSERC/RBC Chair in Data Security in 2019. Dr Kerschbaum's main research interests include data security and privacy in data management and machine learning. He also applies his findings to real-world systems, including databases and supply chain management systems. In 2019, he received the Outstanding Young Computer Science Researcher Award from CS-Can, and was also recognised as a Distinguished Scientist by the Association for Computing Machinery.

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FUNDING

NSERC
Royal Bank of Canada
SAP

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SOFTWARE & SYSTEMS ENGINEERING: INTEGRATING TECHNOLOGY INTO OUR EVERYDAY LIVES

Software is becoming an increasingly important element of our everyday lives – permeating many of the technologies we use regularly. As our software systems become increasingly sophisticated and ingrained into our lives, it is critical to our livelihoods that they remain both functionally correct and easy to use, even as their complexity increases. **Professor Manfred Broy** and his colleagues at the Technical University of Munich aim to ensure a smooth transition to a more software-dependent world, through new advances in the field of Software and Systems Engineering.

Software & Systems Engineering

As digital technologies rapidly improve, they are becoming increasingly integrated with the physical world, and therefore, our everyday lives. The key to the success of these technologies is the software that tells them how to run, and ultimately, determines their functionality. 'Today, software is becoming the most important force in technology,' says Dr Manfred Broy of the Technical University of Munich. 'Therefore, it is key to understand and manage the classical tasks in Software and Systems Engineering.'

These classical tasks can be summarised by their aims to define real-world goals, and the behaviours and limitations of the software in realising them. Finally, it will be implemented by the command sequences that will see these goals achieved into physical hardware, through computer code. Once the software is

implemented, Software and Systems Engineering continues to ensure that its specifications and real-world goals are being met, while managing its evolution over time, and between different systems. In recent years, these techniques have ensured that software continues to run reliably, minimising any potentially disastrous hitches.

A Need for Rapid Improvements

Despite significant improvements in Software and Systems Engineering, Dr Broy believes that they may not be happening fast enough. As the capabilities of new technologies grow in complexity, the software required to carry out tasks in the physical world is now itself growing increasingly large and complex. To ensure that these technologies are reliable for their many millions of users around the world, the capabilities of Software and Systems Engineering will, therefore, need to change with them. As Dr Broy explains,

concerted efforts to develop these systems in a clean methodological way are now needed across a diverse range of current technologies.

'There are a large variety of applications, including automotive systems, avionics systems, production automation, telecommunications, robotics, client-server systems, web-based systems and many more,' he summarises. With so many of us using these technologies every day, Dr Broy now sees the necessity to push Software and Systems Engineering beyond its current capabilities as a problem that quickly needs addressing.



'Today, software is becoming the most important force in technology. Therefore, it is key to understand and manage the classical tasks in Software and Systems Engineering.'



Adapting for Real-World Interaction

In the past, computer scientists involved in Software and Systems Engineering have widely succeeded in their goals to build system and software architectures, implement software using code, and verify the quality of software systems over time. Now, Dr Broy believes that the growing integration of software and physical users calls for more advanced Software and Systems Engineering systems that can capture this interaction. Ideally, such techniques would result in user and system interfaces that ensure technologies are easy to use, maintain, and move between different hardware, while being safe, secure and reliable.

'Since software systems today are mostly embedded into cyber-physical systems as well as global networks, and interact with the physical world including users, it is most important to capture this interaction also in looking at key concepts related to the physical world,' says Dr Broy. In their research, Dr Broy and his colleagues aim to achieve these properties by building a platform for Software and Systems Engineering,

which supports this physical interaction, through the use of computer models that address several key issues.

Developing a System Model

Dr Broy and his team's first step towards achieving this ease of interaction has been to build a reliable foundational model, onto which improvements in Software and Systems Engineering can be easily implemented. The ultimate aim of such a model is to ensure that user interfaces can convey complex systems of software, in ways that make them easy for everyday users to interact with. 'The centre of the work is around a system model which supports all the previously-mentioned aspects by following the key principles of Software and Systems Engineering, such as interface abstraction, encapsulation, information hiding, modular composition, and flexible specification based on a concept of interface and system composition,' says Dr Broy.

As well as this ease of interaction, the model needs to ensure that interfaces can reliably convey what the software is doing to their users, while maintaining

simplicity. At the same time, the model addresses the needs of the developers. 'My work encompasses different styles of modelling such as direct logical modelling of interface behaviour, and the modelling of interface behaviour by state machines,' Dr Broy continues. 'This leads into possibilities to model the key issues of systems.' Ultimately, Dr Broy describes three aspects where these foundational models will be particularly important: creating improvements in system interfaces, devising ways to divide them into subsystems, and building sophisticated system architectures.

Improving External Interfaces

The first of these issues relate to how system functionalities can be improved, by ensuring ease of interaction with its users through external interfaces. 'The function, or feature architecture, describes the functionality of a system in the form of its external interfaces, including the interface behaviour,' Dr Broy says. In this context, 'feature architecture' refers to the high-level structures of computer code that underly the running of software. Just

like real architects, computer programmers need to fine-tune the details of their designs to ensure that their software runs smoothly.

As the only bridge between potentially highly complex software, and the users who likely have no knowledge of its inner workings, the functionality of an external interface is crucial to ensuring reliable system operations. The ‘feature architecture’ that Dr Broy describes, therefore, ensures that interfaces behave in such a way as to simply summarise to the user what the software is doing, while also ensuring that users have access to all of the capabilities of the software.

Defining Logical Subsystems

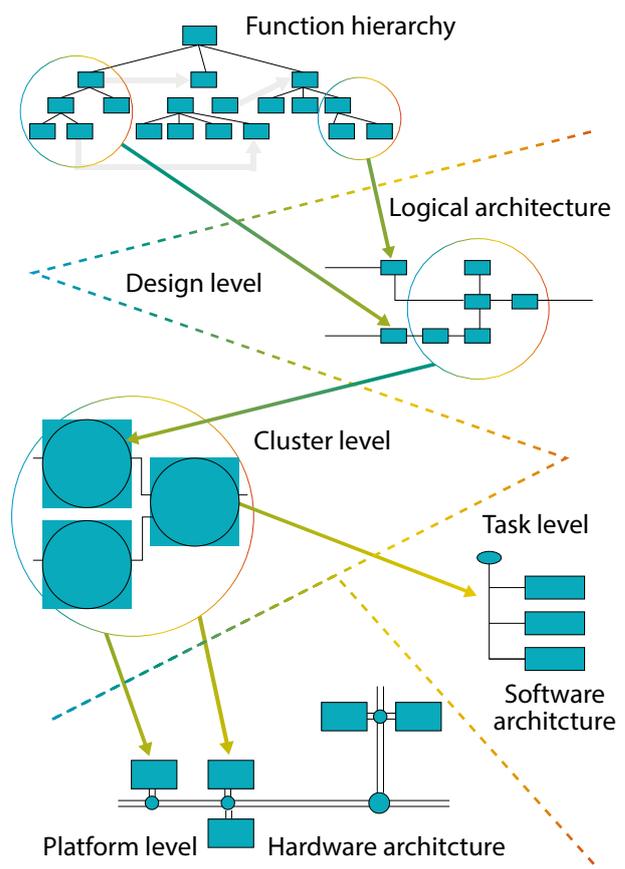
Secondly, Dr Broy’s model acknowledges how complex software needs to be broken down into less complex ‘subsystems’, making them easier to use for developers. ‘Logical subsystems or component architectures decompose a system into a number of subsystems or components which are composed to deliver the required functionality,’ he explains. From the cells in a beehive’s honeycomb to the modular parts of a space station, a wide variety of systems benefit from being broken down into easier-to-manage subsystems, and software is no exception.

If not carried out correctly, however, creating this kind of modular system could be detrimental to the overall system. Dr Broy and his colleagues address this issue by breaking systems down into modules that work together to achieve the goals of the software as a whole. Therefore, their model can turn sprawling software into sets of smaller, simpler systems – making them easier to convey to everyday users through external interfaces, while retaining their capabilities.

Constructing Technical Architectures

Finally, the subsystem architecture ensures that the sequences of events that define the running of the software are carried out without any major issues. ‘Technical architectures consist of hardware, deployment, and scheduling,’ Dr Broy explains. ‘In particular, they consider issues of computational complexity, performance, the technical realisation of such systems.’ Again, in comparison to the work of an architect, ‘technical architecture’ refers to the finely-tuned designs of software applications.

As the physical manifestation of the instructions carried out by software, hardware is a critical element to consider in Software and Systems Engineering. If the system is to function correctly, the software’s commands must be within the capabilities of the hardware. The team’s model, therefore, ensures that hardware runs smoothly during its interactions with users, while maintaining the function of all of the complex tasks required of it.



Bridging the Gap

Through developing these three key architectural views, Dr Broy believes his team’s work will result in improved principles in Software and Systems Engineering – forming a reliable, ubiquitous platform for developing new software. ‘The approach provides the theory for all these issues, and therefore forms the foundation of a comprehensive approach to the development process, the required methods, and tool support,’ he says.

Ultimately, these efforts could ensure that interactive technologies with ever-increasing complexity will continue to be both reliable and easy to use, as we become increasingly dependent on them in our everyday lives. In future research, Dr Broy and his colleagues will focus on improving their models further, with the ultimate goal of making them commercially viable. ‘The next steps will be to bring theory closer to practice; combining it with existing, more pragmatic modelling approaches,’ he concludes.

If the team achieves its goals, the increasingly complex technologies of the future will be able to reliably carry out their vital roles. Even as these systems become increasingly integrated into our everyday lives, future developments in Software and Systems engineering will ensure that complex software can continue to do its work behind the scenes as we interact with it.



Meet the researcher

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Professor Manfred Broy received his PhD in Informatics in 1980 at the Technical University of Munich (TUM), Germany, for a thesis focussing on the transformation of programs running in parallel. In 1983, he founded the Faculty of Mathematics and Informatics at the University of Passau in Germany, where he worked as the dean for several years. In 1989, he moved back to TUM, where he founded the Department of Informatics. Here, he worked as a full professor until his retirement in 2015. Over the course of his career, Dr Broy has achieved numerous awards. In 1994, he received the Leibniz Prize from the German National Science Foundation (DFG) for his outstanding academic achievements, while in 2003, he obtained a Doctor Honoris Causa from the University of Passau. In 2007, he won the Konrad Zuse Medal, which is the highest award of the German Computer Science Society. Dr Broy is a member of the German Academy of Natural Sciences and the German Academy of Engineering Sciences. His main research interests involve the scientific modelling and development of powerful, software-intensive systems.

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SELFIE – SELF-VERIFICATION OF ELECTRONIC SYSTEMS

Electronic systems influence many aspects of daily life. It is imperative, therefore, that these systems are working as intended and expected. The process of ensuring the correctness of systems is called verification. Traditional verification methods, however, are time-consuming, costly, and can hold up production and implementation. To meet this challenge, **Dr Rolf Drechsler** and **Dr Christoph Lüth** of the German Research Centre for Artificial Intelligence have developed a more efficient, in-situ *self-verification method*.

Ensuring the Safety of Electronic Systems

From smartphones to medical appliances, and from transport to the factory floor, electronic systems are everywhere. The computers that drive these systems are incredibly powerful, yet compact. Moreover, multiple electronic systems are often integrated into larger multi-faceted processes. Indeed, the electronic systems with which we interact on a daily basis are very complex.

Managing this complexity is certainly a challenge – yet, it is incredibly important that we do. Not only do people expect their devices to work as intended, they expect manufacturing companies to guarantee the safety of their products. Consider, for example, guidance and safety systems in cars and aeroplanes. A failure in one of these systems could have serious consequences. It is easy to see why, then, they need to function correctly under all possible circumstances.

The verification of electronic systems refers to ensuring this. In order to achieve this goal, a model of the correct behaviour of the system is formulated. We then check that the system as we built it behaves exactly as the model describes it should. However, this is a complicated and time-consuming process, and as electronic systems become more complex, traditional verification methods, which are carried out prior to installation, can become prohibitively expensive. Because of this, full verification is not possible in most instances, leading to systems where critical error cases have been missed out, and which subsequently still contain undiscovered ‘bugs’.

To address this, Dr Rolf Drechsler and Dr Christoph Lüth of the German Research Centre for Artificial Intelligence in Bremen, Germany have developed an in-situ verification method known as ‘Self-Verification of Electronic Systems’, or ‘SELFIE’. SELFIE aims to ensure the safety and efficiency of electronic systems within their real-world settings – saving time and money in the process.



‘Traditional’ Verification Processes

As mentioned above, the verification of electronic systems refers to ensuring that they are functioning correctly. It typically occurs *before* the production and implementation phases. By means of verification, designers can check: (1) whether the system is free of errors, (2) whether it meets its specified requirements and (3) whether it shows some unintended behaviour. Verification is not to be confused with validation, which determines if



the system is suitable for the chosen application. In other words, verification checks if we have built the system correctly, whereas validation checks if we have built the correct system.

There are three common verification methods – simulative, emulative and formal verification. Simulative verification is based on a *model* of the system. The inputs are explicitly assigned and put through the model, and afterwards the outputs are compared to the expected values. However, there are so many different combinations of input values that we typically cannot cover all of them during verification. Emulative verification is like simulation; however, it is carried out using a true prototype of the system. It is faster, but it still will not cover all possible inputs. Formal verification formulates the correctness question as a mathematical proposition, which is then to be proven. This covers all possible inputs, but as of today, it only works for small or medium-sized systems.

Why Traditional Verification Methods Are Inadequate

According to Dr Drechsler and Dr Lüth, more than 40% of the time and costs associated with the design process are devoted to proving the correctness of a system. If the verification process is delayed and does not produce the desired outcome, then precious time and funds are on the line. They also highlight that, while a few years ago the actual implementation process was the core activity in any design flow, verification dominates the design process today. Moreover, the time and money spent on verification could be used to add new features to the system or improve it in some other way.

There is another limitation, which stems from the fact that designers often terminate the verification process before functionality and correctness can be ensured. However, taking shortcuts frequently allows ‘bugs’ or faults to persist into the final product. These bugs can often prove costly in terms of performance issues and maintenance costs. In some cases, they could later prove to be unsafe.

SELFIE Seeks to Address These Limitations

Up until now, research in the field of electronic system verification has failed to address these problems satisfactorily. In many cases, this is because the research and suggested solutions are based on pre-existing methods, that is, simulative, emulative and formal verification. As a result, not enough advancement has been made and the problems persist. Therefore, a new, fundamental approach was urgently needed. To address the issues, Dr Drechsler and Dr Lüth developed the SELFIE methodology.

The SELFIE methodology enables the system *itself* to eventually complete the verification. The emphasis is on *in-situ* verification *after* deployment. The methodology, in simple terms, is based on having a dedicated verification system, which is separate from the target system. It is made up of hardware, software and integrated components that work together to take measurements, compare them to expected values, and provide verification reports – with all this



occurring simultaneously during run-time in its unique operational context.

What SELFIE Offers

Ultimately, by extending the time to market, SELFIE saves time and money. Of course, safety-critical requirements must still be covered prior to production, but instead of simply terminating the verification process after that, verification can continue after production until completeness has been achieved. Moreover, the information acquired from the system in its 'real-world' environment allows, in many cases, the verification to go through easier and in less time.

In summary, as Dr Drechsler and Dr Lüth explain, self-verification in the actual operating environment significantly simplifies the verification task. This enables a more application-specific consideration and, therefore, not only improves the effectiveness of the verification but also the quality of the results.

A Case Study – Smart Home Control System

As a starting point, Dr Drechsler and Dr Lüth examined the validity of SELFIE using a simple case study. The case study consisted of a light controller supporting multiple light sources, luminosity sensors, manual switches and presence detectors. Such a system would be typical in a 'smart' building that aims to control the use of artificial light in relation to natural, ambient light. Dr Drechsler and Dr Lüth felt that this was an excellent system to assess SELFIE with.

In the associated paper, they noted that home-automation systems like these are designed in a flexible fashion, so that they can be applied in various contexts. Hence, to verify the correctness of the system, designers and engineers need to check all possible configurations, for all possible deployment contexts, even if they may never be applied during the system's

lifetime. A post-production approach that verifies the system in its operational context, however, ensures that only the relevant parameters are checked. In summary, Dr Drechsler and Dr Lüth validated SELFIE during this study. SELFIE allowed the verification of a system that was previously out of reach using contemporary tools and methods, and proved to be much more effective and efficient.

Where to From Here?

Dr Drechsler and Dr Lüth acknowledge that self-verification does not necessarily replace pre-existing verification processes. At the very least, however, it will enhance them. They explain, 'we may use all well-known powerful tools at design time to prove verification conditions as before, and still use verification after deployment to tackle the verification conditions we could not prove during design – giving us the best of both worlds.'

The next step is to establish SELFIE's applicability and value in relation to more complex smart systems that combine more technologies such as safety, security and climate control. They also desire to explore the following questions: What can be done if SELFIE fails to verify the system? Could self-repair be incorporated? They also want to investigate how to fit self-verification aspects into existing design flows, and how self-verification impinges on or changes the overall design process.

The central goal of the SELFIE project is to bring about a fundamental change in the development of electronic systems. Instead of having to finish the verification before delivery regardless of success, systems will verify themselves during operation. This self-verification process will ultimately save engineers and technicians time and money, and deliver more value to the customer. It may also have follow-on effects in terms of ensuring a system's performance and safety – a welcome improvement as the electronic systems on which we rely every day become more pervasive and complex.



Meet the researchers

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Dr Christoph Lüth received his PhD in 1998 from the University of Edinburgh. He then joined the team at Universität Bremen (the University of Bremen), serving as Associate Professor and Lecturer. Whilst continuing to work at the University of Bremen, Dr Lüth also joined the German Research Center for Artificial Intelligence in 2006, where he is now the Vice Director of the Research Department for Cyber-Physical Systems. His research covers advanced software development – from the theoretical foundations to the development of tools to construct and verify software.

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Dr Rolf Drechsler received his PhD in computer science from the Johann Wolfgang Goethe University, Germany, in 1995. After various postings in both industry and at educational institutions, he joined the Institute of Computer Science at the University of Bremen, Germany in 2001. He currently serves there as Professor and Head of the Group of Computer Architecture. In 2011, he also joined the German Research Center for Artificial Intelligence in Bremen, where he serves as Director. His current research interests include the development and design of data structures and algorithms with a focus on circuit and system design.

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FUNDING

Ministry for Education and Research (BMBF), grant no.
01IW16001



PAMELA: INTEGRATING MODELLING AND MACHINE LEARNING FOR AUTONOMOUS ROBOTICS

Machine learning is rapidly advancing the decision-making capabilities of today's computers, yet without an in-depth knowledge of the programming it involves, many engineers and researchers find current technology inaccessible. **Dr Paul Robertson** at Dynamic Object Language Labs (DOLL) in Massachusetts believes that a solution to the issue may have been hidden in plain sight: machine learning itself. His ideas have now culminated in 'Pamela': a universal, open-source language capable of modelling real-world systems, and building plans to overcome challenges. The language and its related tools could soon open up significant opportunities in the emerging field of artificial intelligence.

Machine Learning

Until very recently, the human mind has remained the only decision-making system smart enough to operate the many systems we use to keep our civilisation ticking. To deal with the intricate webs of interconnected variables that link systems together, and to their surrounding environments, our intelligence has so far been critical to making the complex, rapid decisions needed to keep them functioning.

Yet this picture is now changing quickly with the emergence of artificial intelligence (AI), which uses algorithms to first learn about systems and their surrounding environments, and then to make useful decisions about their operation.

'Systems ranging from photocopiers to spaceships are designed by human engineers,' explains Dr Paul Robertson of Dynamic Object Language Labs (DOLL), a Massachusetts-based

company. 'Unlike the messy natural world, they can be described accurately and fairly completely. By turning knowledge of their engineering into models and having those models as part of the runtime system, systems can use AI reasoning to intelligently diagnose and operate such a system.'

Known as 'model-based autonomy', this area of research has exploded over the past 15 years. However, Dr Robertson acknowledges that a significant barrier lies in the way of the technology's widespread adoption.

Bridging the Gap

To apply machine learning in the real world today, researchers must first build models of the systems it will be applied to. These essentially consist of sets of variables, each associated with their own probability distributions, which approximate the characteristic behaviours of systems in different conditions. Subsequently, data gathered



by a system's sensors are linked to a separate 'solving' program, which uses models to make smart decisions about the system's operation.

The lack of an appropriately expressive modelling language has forced researchers to make do with simple models, seriously limiting the advances



in autonomous systems and machine learning. So far, this problem has delayed the many potential benefits of machine learning, especially for real-world systems, but Dr Robertson believes that a solution has been hiding in plain sight all along: machine learning itself. Instead of manually building models and writing the tedious programs required to link them with solving languages, he proposes a language and toolchain that together are capable of building models themselves, using only sensor data.

Understanding the Open World

To lay the groundwork for this new language, Dr Robertson and his colleagues first needed to consider how an AI system should deal with the complex realities it experiences through its sensors. Instead of executing actions based on fixed prerequisites, as most pre-programmed robots do today, more intelligent robots must consider a range of possibilities when making decisions about their future actions, based on the patterns they observe. 'As we relax the constraints on our models, we move towards systems that can be observed to exhibit certain regularities, and thus, their models can be learnt by AI,' explains Dr Robertson.

This behaviour is comparable to how wild animals learn how best to survive given the conditions of their habitats and the capabilities of their bodies.

'It allows us to change our models in the face of new evidence,' Dr Robertson continues. 'This finally leads to exploration and learning rather than engineering design. As modern AI systems venture out into the world, as robots, they need as much of the reactive learning found in primitive animals as they do for high-level reasoning. Furthermore, they need to learn by themselves.'

Introducing Pamela

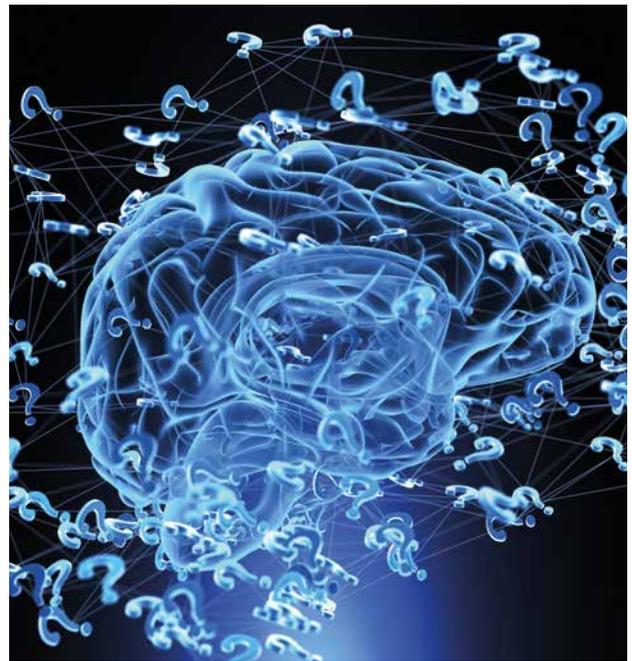
This line of reasoning has now culminated in a new modelling language, named 'Pamela', developed by Dr Robertson and his colleagues at DOLL. In contrast to previous modelling languages, Pamela was designed to work with state-of-the-art machine learning and planning tools designed to operate in the real world. In this case, the probability distributions of each variable in a model themselves can be modelled by Pamela. 'These "probabilistic variables" allow us to reason over uncertainty in models, and an autonomous system's beliefs about them,' Dr Robertson explains.

For the first time, this brings the two worlds of modelling and probabilistic programming together into a single, unified language. 'Pamela was developed to add probabilistic variables and probabilistic reasoning to model-based systems,' Dr Robertson continues. 'Finally, the models themselves can be learned, and the learned models can change as learning makes them more reliable.'

Applying a Model

In their latest research, the DOLL team has developed a toolkit for applying their language to real-world situations, named the 'Pamela Autonomy Toolchain' (PAT). To explain how it works, the researchers describe a simple problem in which a robot is low on battery and must find a charging point to plug itself in to. The charging point is locked, however, and the robot must first find the key to unlock it somewhere in the room. To achieve this goal, PAT first builds a five-stage plan: go to the key; take the key; go to the charger; insert the key; and start the charge.

To enact these steps, several parameters must first be set out in a model of the situation. For example, if the robot is close to an object, then it can pick it up; and in order to move the key, it must first be holding it. With machine



learning, the physical actions associated with each of these parameters can be learnt through experience. However, through previous approaches, researchers needed to establish the instructions for this themselves. With PAT, on the other hand, the probabilities of the variables measured by the robot's sensors can be used as the variables required to build a realistic model of the situation, with no human input required.

Updating Belief States

Dr Robertson first illustrates how this would be done in current approaches to machine learning. 'The robot believes that there is a key on one of two tables, based on prior history, but the probability of the key being on any one of the tables is low,' he says. 'Therefore, it plans to get close enough to one of the tables in order to increase the certainty in a key being there. The closest table has the least cost, so it will probably be picked.' When it is close to the table, the robot will then either confirm that the key is there or change the probability of it being there to zero. In this case, it will move to the second table and repeat the process.

More realistically, however, the key may not be on either of the tables, but could be placed anywhere on the floor, making the situation far more complex. 'If you have to search for the key before proceeding, it is clear that the whole plan cannot be produced in advance,' continues Dr Robertson. 'A highly contingent plan that covers every possibility of where the key might be would be a very complex plan. In this kind of situation, the robot needs to take actions to improve its knowledge about the world, and it also needs to take actions to complete its mission.'

This can be done through PAT, which establishes a set of 'beliefs' about the actions a system must undertake to realise

the parameters of its plan, by assigning higher or lower probabilities to them. Therefore, the robot learns to look around the room in order to improve its belief state, allowing it to assign higher probabilities to the key being in particular areas. When its task is complete and the robot finally plugs in, a 'reward' system adds value to each step that successfully contributed to the overall goal. This means that in future runs, the robot will believe more strongly that the key will be in a similar area to where it was before, reducing the need for planning. Ultimately, this equates to a more reliable model of the situation than a human researcher could ever build.

Engaging with Research Groups

Having established a rigid framework for Pamela, Dr Robertson and his colleagues at DOLL are now starting to encourage members of the wider programming community to make their own contributions to the language. Since Pamela is now available online as open-source software, the team strongly hopes that its capabilities will quickly grow and evolve through the inputs of specialists around the world. If realised, this could bring about new machine learning algorithms, better planning systems, and new systems for diagnosing problems when plans are derailed.

With the diversity of expertise afforded by this approach, Pamela could soon equip researchers and engineers across a wide range of fields – including those with little knowledge of the language used in machine learning – to apply their models in the real world. With future research, Dr Robertson's team hopes to integrate their 'Continuous Effective Robot Learning' (CARL) platform, which they first developed in 2019. If added to PAT, the team believes that CARL would help make autonomous systems more independent. The level of human involvement in AI systems is one of today's greatest challenges.



Meet the researcher

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Dr Paul Robertson holds a DPhil from the University of Oxford, for a research project entitled 'A self-adaptive architecture for image understanding'. Since then, he has worked at numerous prestigious institutions and companies, including the University of Massachusetts at Boston, the University of Texas at Dallas, Artelligence Inc, Symbolics Inc, Massachusetts Institute of Technology, and BBN Technologies. He has had a lifelong interest in reflection in intelligent systems, and the role that reflection can play in adapting responses to changes in the environment. A key interest has been advanced planning, especially in the context of self-adaptation. Today, Dr Robertson's research at Dynamic Object Language Labs (DOLL) Inc centres around the role of emotions and consciousness in robotic systems as a natural extension from his earlier work on reflection and self-organisation.

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FUNDING

This work was supported by Contract FA8650-11-C-7191 with the US Defense Advanced Research Projects Agency (DARPA) and the Air Force Research Laboratory.

FROM MACHINE LEARNING TO MACHINE UNDERSTANDING

Despite dramatic advances in neuroscience and biology in the 20th and 21st centuries, our understanding of the brain remains very limited. **Dr Yan M Yufik**, Head at Virtual Structures Research Inc, USA, is a physicist and cognitive scientist who has spent over 20 years combining experimental findings and theoretical concepts in domains as diverse as neuroscience and thermodynamics to form a theory of the brain. His focus has been on elucidating the mechanisms underlying human understanding and applying the results to the design of machines that can not only learn but understand what they are learning.

What is Machine Learning?

Artificial intelligence (AI) is concerned with designing computing machines that can replicate or even amplify human cognitive capacities. Recent news has been awash with examples of artificial intelligence that seem to come straight from science fiction, including self-driving cars, facial recognition, and virtual assistants such as Siri and Alexa. AI approaches are abundant in military applications and can also be found in less obvious places, powering algorithms used by online marketing companies, social media websites, financial institutions, and medical diagnostics.

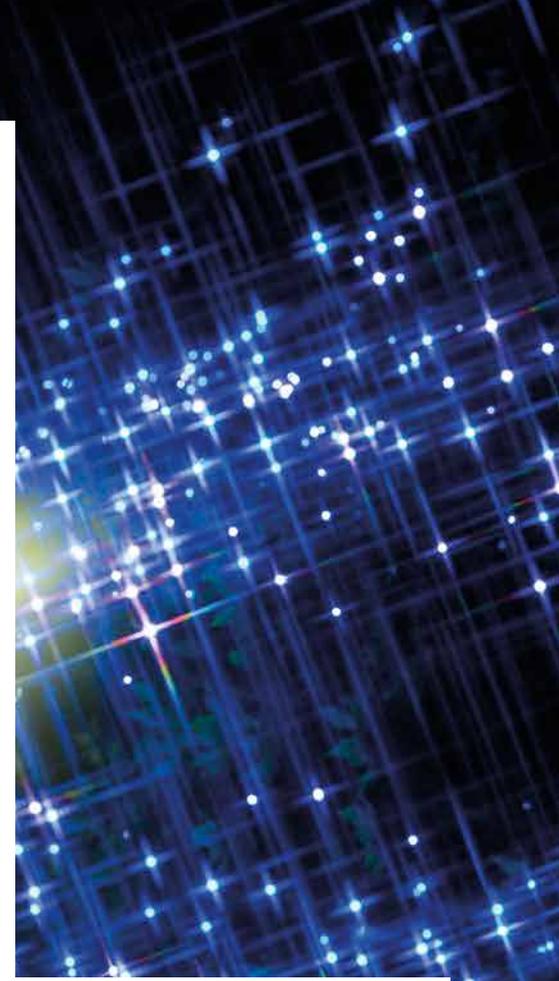
These accomplishments are due to advances in machine learning, built predominantly on the idea of neural networks that originated in the middle of the last century. Three factors contributed to the success of this idea: large financial investment in the development of learning algorithms, recent theoretical breakthroughs in the development of these, and nearly a billion-fold increase in the efficiency of computing devices.

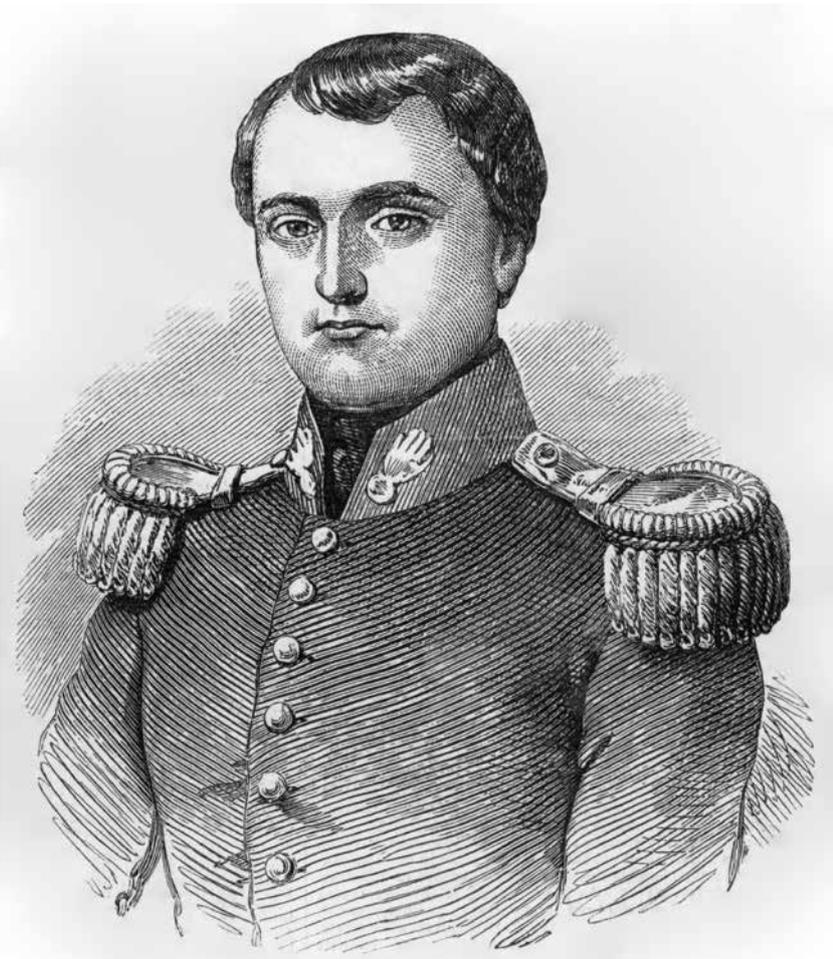
This increase in the efficiency of computing devices was critical: machine learning demands massive amounts of computation. The implementation of neural networks began around 1960 using the computers available at that time. Matching computing power available today for \$500 to that available back in 1960 would require an array of 1960-type computers at the cost of about \$9 trillion (adjusted for inflation). The development of AI technology has relied on the rapidly increasing efficiency of computing machines. Dr Yan M Yufik, Head at Virtual Structures Research Inc, USA, argues that the development of human intelligence followed a path orthogonal to that pursued in AI.

Machine learning employs a variety of statistical learning methods. Despite some differences, all these methods are based on the same principle: learning in the absence of understanding. Take, for example, a database of medical records containing data about conditions and the corresponding diagnosis in a multitude of patients. Machine learning can determine patterns in

the data allowing the machine to make responses to combinations of conditions that would appear to represent meaningful diagnostic decisions. In principle, the same learning algorithms can be applied to a database holding records of chess games, allowing the machine to produce responses to chess positions having the appearance of meaningful moves. However, in both cases, learning was concerned only with determining patterns in the arrays of symbols and was oblivious to meaning: no explicit knowledge of diseases or chess rules and strategies has been entered into the machine.

Learning algorithms make it possible to train machines to respond adequately to different inputs while being clueless about the meaning of either the inputs or the responses. For many people, the prospect of 'clueless' machines is a frightening one, especially if they are delegated important decisions with life-or-death consequences, as in medical treatment, car driving, or weapons control.





According to Napoleon, 'the art of war consists, with a numerically inferior army, in always having larger forces than the enemy at the point which is to be attacked or defended.' As per Dr Yufik's theory, thermodynamics enforces 'Napoleonic strategy' in the evolution of the brain: mechanisms are formed allowing allocation of neuronal resources sufficient for dealing successfully with a growing variety of changing conditions while, at the same time, minimising energy expenditures incurred in the operation of those mechanisms. This evolutionary development culminated in the mechanisms of mental modelling in humans (for example, understanding situations in a battlespace requires constructing models capturing fluid relations between battlespace entities. Successful models enable the commander to plan anticipatory deployment and manoeuvring, as required by Napoleon's winning formula)

For the past 20 years, Dr Yufik has pioneered research in the field of machine understanding. His objective is to design machines endowed with a degree of understanding that is sufficient to enable them to carry out complex tasks under novel and unforeseen conditions and to explain their actions and decisions in a manner that is comprehensible and compelling to human users. Reciprocally, he believes that such machines should be able to accept user feedback in a format meaningful to humans and apply it directly when organising their internal processes.

What is 'Understanding'?

Learning is crucial for survival. Even the simplest of organisms can associate conditions with responses and consequences such that when conditions recur, the beneficial responses are reproduced, and the harmful ones avoided. Learning serves well for as long as the conditions recur but fails when they change. Such failures can be particularly damaging if the learned behaviour persists after the changed conditions start penalising responses that were previously rewarded.

According to Dr Yufik, human understanding is an adaptive mechanism serving to overcome the inertia of learning, which includes the ability to timely detect and prioritise changes, allowing the construction of responses to unfamiliar conditions. Understanding is the product of brain activity (i.e., thinking, mental modelling) that is temporarily decoupled from sensory inputs and involves selecting and re-combining memory elements to form new structures (mental models) that help us to both anticipate future changes and accommodate the unanticipated ones.

While learning is tied to past experiences, understanding can deviate from them. Take, for example, the earliest known artefact dated approximately 30,000 years BC which is a figurine depicting a creature with a human body and lion head. Perhaps, imagining such creatures expressed a primitive understanding of important realities, serving a dual purpose of indicating the possibility of encountering opponents with extraordinary (lion-like) strength and ferocity, and allowing advance preparation for such encounters. From imagining chimeric creatures to imagining and designing intelligent machines, the process of understanding involves selective adjustment and re-combination of previously formed memory structures to produce new ones.

Meaning is imputed to such combinations when relations between components are apprehended: first, behavioural repertoires are attributed to memory elements representing objects, followed by imagining how the behaviour of one object can impact the behaviour of other ones. Imagine, for example, a drawing depicting a vase lying on the floor next to a stand and a cat sitting nearby. Imagining a cat jumping and knocking the vase down imputes meaning to the drawing which would have otherwise remained a meaningless aggregation of objects. Note that neither the jumping cat nor



Carl Friedrich Gauss, one of the greatest mathematicians of all time, surprised his teacher in elementary school when quickly adding integers from 1 to 100. While the other students were laboriously moving along the number row, young Gauss grasped the relations across the row ($1 + 100 = 101$, $2 + 99 = 101$, and so on) thus reducing computing the sum to finding the product of 101×50 . Thus, using mental models to capture global relations in the number series yields the problem solution more quickly and less laboriously.

the standing vase is in the drawing, and that cats usually do not attack inedible stationary objects, so the imagined behaviour is a product of adjustment and re-combination rather than merely a recollection of past experience.

The importance of mental modelling has been long recognised in cognitive psychology, but Dr Yufik proposes a specific and central role for it in his theory. Note that you have probably observed different forms of cat behaviour (climbing, running, sitting, jumping, lying on a side, sleeping, reaching, eating, and so on) but images of a sitting cat floating through the air and hitting the vase or other such choices were unlikely to cross your mind. Dr Yufik hypothesises that mental models are synergistic memory structures where all components are amenable to mental variation and are all mutually constrained and coordinated. Such mutual constraining has the dual effect of limiting the range of plausibly imaginable variations and causing co-variations across the structure consistent with any local change. For example, if you imagine varying the height of the stand, your image of plausible cat behaviour will vary accordingly.

The experience of attaining understanding accompanies the formation of mental models where cross-coordination between all components radically reduces the number of degrees of freedom available to them. These benefits of understanding might not be apparent when dealing with a few objects but become obvious in multi-object situations affording many choice combinations, such as in playing chess or fighting battles. Chess machines have to reach the speed of hundreds of million decisions per second in order to compete with humans capable of at most a few decisions per second. Master players compensate for the disadvantage in speed by forming synergistic models of chess positions that confine the analysis to, figuratively, a hair-thin path in the combinatorial space the size of the Pacific Ocean. As a result, bad moves are kept outside such analytic paths and do not come to mind in players who understand the game (no more than illegitimate moves would come to the mind of novices familiar with the rules) while the way forward can be envisioned to a substantial distance (e.g., the astonishing 15 moves 'look-ahead' analysis reported by chess champions).

Step-by-step computing (analysis) is time- and energy-demanding while cross-coordination in mental models is simultaneous and computation-free and, thus, energy-inexpensive. Embracing a physics perspective, Dr Yufik argues that thermodynamics enforces energy efficiency in neuronal systems, and thermodynamic pressure propelled evolutionary transition from protohumans (a hypothetical prehistoric primate) to humans with a desire to understand themselves and their world.

According to Dr Yufik's theory, the basic functional units in the brain are not neuronal networks but neuronal packets which are groups of tightly associated neurons underlying the perception of objects. Inducing different firing patterns inside packets underlies apprehending and imagining behaviour variations (e.g., imagining a sitting, running, or jumping cat involves inducing different firing patterns in the 'cat packet'). Dr Yufik further proposes that apprehending relations between objects involves establishing co-ordination between successions of firing patterns in the corresponding packets. Packets form as a result of self-organisation in associative networks, not unlike the formation of raindrops in water vapour. Energy barriers at the packet boundary (again, not unlike boundary surfaces in raindrops) make packets stable and amenable to composition into models. Crucially, forming coordinated compositions of packets and manipulating them is more energy efficient than manipulating individual packets.

While Dr Yufik's ideas are speculative, modern experimental techniques have started delivering data that seem to support them. His theory has also led to conclusions consistent with a principle of brain operation advanced recently by Professor Karl Friston, asserting that processes in the brain are driven towards minimising surprises. In a joint paper, Dr Yufik and Professor Friston argue that principles of surprise minimisation



In the now-famous experiments, American psychologist Edward Thorndike placed hungry cats in cages equipped with a lever for opening the door. When frantically thrashing around, cats would accidentally push the lever and thus free themselves. After a series of repetitions, cats would learn the requisite action and, when placed in the cage, proceed to push the lever without delay. However, when one of the sides in the cage was removed, the trained cats would still implement the lever-pushing routine instead of simply walking out. Cats were learning – but failed to understand either the situation or what they had learned.

and energy cost minimisation are mutually consistent and complementary: pressure to reduce energy costs sculpts and fine-tunes mental models so that more reliable predictions are produced diminishing future correction costs. Discovering the dual benefit of packet coordination by the evolution (more accurate and reliable predictions at lower energy costs) may be responsible for the emergence of sapience about 100, 000 years ago.

According to Dr Yufik, the gradual build-up of sensory-motor coordination machinery in the brain could plausibly have brought evolution to the point where a one-step transition from protohuman to sapience was possible. Think of walking and carrying a cup of hot coffee in one hand and a pile of documents in the other: the process requires precise dynamic coordination of multiple muscle groups to avoid spilling the coffee and or the papers. Imagine reaching a door and trying to open it: the coordination pattern needs to be quickly re-organised to meet the challenge. Dr Yufik's hypothesises that the machinery of sensory-motor coordination in manipulating external objects richly developed in the protohuman was co-opted and re-purposed for manipulating internal 'objects'. And with that, understanding appeared on the scene, enabling advances in technology at a blistering pace: from improving gadgets for throwing projectiles to hit distant objects to designing space craft capable of reaching the moon.



The Gnostron Framework and the Future of Machine Understanding

We should bear in mind that Dr Yufik's theory does not align fully with mainstream AI. The neural network approach argues that intelligence derives from pattern recognition while the neuronal packet approach proposed by Dr Yufik derives intelligence from pattern coordination. Critically, the former makes predictions by extrapolating from the past while the latter derives predictions from understanding the past.

Nonetheless, Dr Yufik proposes that the approaches are not mutually exclusive and can be integrated within a unifying mathematical framework. The neuronal packet approach has been expressed in architecture and mathematical formalism dubbed 'gnostron' (which is different from and complementary to 'perceptron' formalism and architecture that initiated the development of neural networks).

Perceptron architecture includes a fixed set of interconnected neurons (i.e., a neuronal network) while gnostron processes operate on a neuronal pool, selecting and combining neurons into packets and packet compositions (models) that can be tried out and then matched dynamically against the streaming input. The process allows dynamically optimising responses in complex situations, as in the battlespace where conditions are fluid and never twice the same.

Application of the gnostron framework in machine understanding is in the early stages, requiring mathematical and, possibly, hardware engineering approaches different from those currently employed in AI. These developments aspire to deliver a new generation of AI systems capable of carrying out complex tasks on small energy budgets and in a manner the users can trust and understand. Such systems will be able to envision immediate and distant consequences of their actions and explain their decisions in terms relevant to both internal operations in the machine and human understanding: values, objects, behaviours, and relations. Developing machine understanding is a worthwhile challenge: the distance between future AI and its present version cannot be less than that between humans and their evolutionary ancestors.



Meet the researcher

Dr Yan M Yufik

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Dr Yan M Yufik holds a PhD in physics and received postdoctoral training in cybernetics and cognitive science. Dr Yufik currently heads Virtual Structures Research Inc, a non-profit company that aims to facilitate the study of biological and artificial intelligence. Along with colleagues, Dr Yufik is pioneering the field of machine understanding, an area of artificial intelligence that uses biophysics and neuroscience approaches to simulate human understanding in artificial systems. He holds five US patents and has published numerous papers and several book chapters on the subject.

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Professor Karl Friston, University College London

FUNDING

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THE GAMIFICATION OF BUSINESS PRODUCTIVITY AND SCIENTIFIC EDUCATION

It is undoubtable that virtual reality and augmented reality will soon be an integral part of our daily lives at home, in education, and at work. Here, we look at some of the exciting projects that **Dr William Hurst** of the Department of Computer Science at Liverpool John Moores University is driving forward and read how he is embracing virtual reality and augmented reality to enhance teaching and education, providing insight into how such technology may be utilised in the not too distant future.



The VR panda teddy bear avatar used during proton therapy

Virtual Reality and Augmented Reality

Virtual reality (VR) and augmented reality (AR) have increased in prominence and public interest in recent years, leaping from the pages of science fiction into our homes and workplaces. Although still perhaps seen more as a novelty or a 'must-have gadget' at present, with ever-faster computing speeds and capacity, the future of VR and AR has the potential to become routinely embedded as an enhancement to all aspects of our domestic, educational, and working lives.

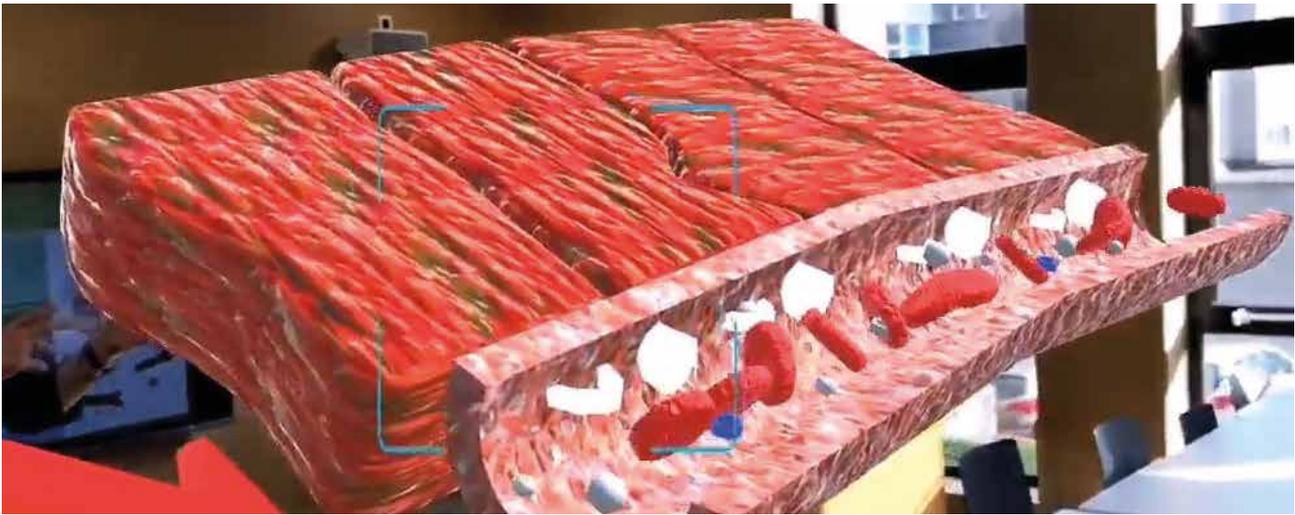
VR and AR differ in several ways. VR is a computer-simulated 3D-environment in which the user wears a bulky headset over their eyes, to become fully immersed (at least visually) in a different virtual environment. The user can interact with and navigate through the often stunningly realistic virtual world, but as a downside, they are effectively cut-off from the real world until they remove their headset or switch off their VR app again.

In comparison to VR, augmented reality allows the user to remain in the real world, aware of their surroundings and those around them but superimposes 2D or 3D computer simulations in real-time onto their field of vision, perhaps through transparent visors or spectacles, to add animations or layers of useful or contextual information.

Preparing for Industry 4.0

Dr William Hurst is dedicated to the development of new technologies to support the transition of the UK's industry into the new manufacturing paradigm – industry 4.0. The fourth industrial revolution is the next stage of manufacturing; taking us into a new phase of autonomous systems driven by access to vast quantities of data and machine learning. The UK has a lower productivity record in comparison with its worldwide competitors, and so productivity-enhancing systems are critical to the nation's future success.

In light of this, InnovateUK funded a project in this area, called Productivity Accelerator (ProAccel). The £102,000 ProAccel project, led by Dr Hurst, was a business and community-centric



AR Molecular Interaction.



Dr John Barrow, Aberdeen University, UK

modular cloud-based multimedia platform. It utilised advanced data analytics and gamification techniques, like AR and VR, to dramatically improve the way productivity information is utilised so that it can support businesses in the new digitally oriented world.

Amongst the prototype's early test applications, the team tested a prototype tower crane cockpit simulator to improve the productivity of training of crane operators, enabling them to learn in a safe but highly realistic 3D virtual environment.

The VR Proton Beam Therapy Unit

Dr Hurst's current research includes several collaborative projects exploring the use of creative VR and AR technologies to augment or revamp current ways of working, with a particular focus on medical and educational settings. An exciting example of this creative approach is Dr Hurst's joint work with Kieran Latham, and Imagin3D of Daresbury Laboratories in Warrington, to create a virtual reality proton beam hospital therapy unit. This work originated through an innovation award to explore the use of AR and VR to increase the productivity of UK businesses. The technology the team has produced has both productivity-enhancing and humanitarian benefits.

Two new hospital-based proton therapy centres have been built in the UK to aid the treatment of different types of cancers and are particularly useful for childhood cancers. The proton beam treatment process, however, can be an intimidating and frightening experience for children as it involves lying inside a large spherical machine for a prolonged period while radiation is directed towards their tumour cells to destroy them.

Children are typically allocated a two-hour time slot to receive their proton therapy treatment; but often this may be insufficient, as significant time may be required to reassure the understandably apprehensive child to enter the machine for treatment, and to remain still throughout the process. Clinical schedules may overrun, or treatment may not be completed if the child is uncooperative. The team have addressed this challenge by developing a VR application that allows children between the age of 3 to 11 to experience the proton beam unit's processes and preparation for treatment, initially through a VR experience. A VR panda teddy bear avatar is used to engage with the child and reassures their anxieties as they are guided through the proton beam therapy process.

While the idea is simple, the VR development process, working with a building information model (BIM), is highly complex. In brief, BIM is the



The team at Imagin3D

process to recreate a detailed 3D model of a real-world object or environment, using 3D scanners to create point cloud data. In fact, such scans are often too detailed for VR use, comprising close to a five million polygon resolution, and so much of the app's development is to manually simplify the scanned models, removing superfluous details by hand. The optimisation process results in a much lower polygon count model that is suitable for deployment into a VR game engine. The proton beam therapy unit VR application is being developed with Unreal Engine software that places the digitised model into a physically dynamic and realistically textured environment. It allows the application of industry-standard gaming models to achieve game-play levels of responsiveness for users.

Augmented Reality for Undergraduate Teaching

Dr Hurst has also recently worked on the development of an award-winning idea (awarded best paper at VISUAL2019), to use augmented reality to enhance life-science education. Led by Dr John Barrow at Aberdeen University, the project aims to develop experiential learning methods using AR cutting edge gaming technology to improve undergraduate teaching.

Dr Barrow's interest is directed towards modernising the way life-sciences are taught at university. Dr Barrow's experience of teaching bioscience and medical students over many years has led him to the conclusion that students often struggle to grasp the complex and abstract nature of molecular interactions and structures within biochemistry and cellular biology. Traditional teaching methods and textbooks have relied on rote learning and static two-dimensional cartoons or symbolic line representations of what are in reality, highly dynamic processes that are hard to then visualise in three dimensions.

Working with Dr Hurst and Imagin3D, Dr Barrow was keen to apply gamification techniques to create more suitable teaching material for the digitally literate generation of students. Gamification is where aspects of gaming technology and approaches are used in a non-game context. In addition, AR

could be used to visually bring to life molecules and cellular activities as part of the classroom experience, and to offer new and engaging learning experiences that move away from purely didactic teaching.

Dr Barrow initially developed his software with Imagin3D and Dr Hurst to explain the complex metabolic processes in insulin signalling and will follow this up with a programme to visualise the glycolytic pathway, the biochemical process in the body to breakdown glucose for the production of energy. Both are fundamental to the teaching of cellular metabolism but are often taught in a linear fashion following the breakdown of one molecule to another in the pathways, a slightly dry and didactic process ripe for a modern make-over.

Student interns were involved to develop gaming aspects of the software with built-in challenges and problems to solve. For example, the students used game animations to build proteins through multiple pathways. The software development was focussed on utilising existing 3D molecular visualisations that are freely available online. These can be integrated into virtual environments, where the user can then interact and 'play' with them in a live situation to help them more intuitively understand their functions.

While this technology is still in its infancy, the potential for its wider use is enormous. The developed learning apps can be deployed digitally through VR, AR, platform-free videos and apps, as well as online. Medical applications could be used, for example, for health professional and patient education, to convey complex ideas or explain treatment procedures.

The Future of VR and AR

The integration of VR and AR into our daily lives will ultimately become a seamless part of our perception of the world around us within just a few decades. Dr Hurst's work demonstrating the wider uses of the technology provides insight into the many potential benefits to humankind in the fields of medicine, education and beyond.



Meet the researcher

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Dr Hurst is a Reader (Associate Professor) in Creative Technologies in the Department of Computer Science at Liverpool John Moores University (LJMU). He has over 60 international publications in the areas of Data Visualisation, Artificial Intelligence, Machine Learning, Computer Graphics and Data Science. Dr Hurst has also had successful grants from the EPSRC, Innovate UK, SBRI and UKAIS for multiple projects within these areas.

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The team at Imagin3D have over 12 years' experience in 3D and immersive technologies, including Augmented/Virtual Reality and Serious Gaming. Imagin3D have produced 2 award winning immersive training environments and delivered the first Virtual Factory on the £20m pilot for the governments 'manufacturing made smarter' scheme. In 2019, Imagin3D were shortlisted for the Halton Chamber New Business of the Year and won two academic best papers for their work in AR and VR field.

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FUNDING

Productivity Accelerator (ProAccel) – InnovateUK/SBRI funding, £102,000 – code: <https://gtr.ukri.org/projects?ref=971582> – Project Reference: 971582

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ENGINEERING



SOLVING SOCIETAL CHALLENGES THROUGH INNOVATIONS IN ENGINEERING

Our third section highlights a fascinating selection of innovations across diverse fields of engineering, from developing sophisticated robotic assistants to monitoring and predicting natural disasters.

First up is John Mackay and his team at Progeny Systems Corporation, who are developing Earth-based hardware that works in a similar way to the networks of satellites used for global navigation. The company's technology could provide a crucial yet inexpensive alternative to GPS technology, safeguarding against outages.

In our second article of this section, we meet Dr Paul Robertson, Chief Scientist at Dynamic Object Language Labs in Massachusetts, whose research also appeared in the computer science section of this edition. In this section, however, we showcase his work in developing robotic assistants, with a particular focus on those designed to aid repair missions. By considering how robots can be programmed to recognise tasks and comprehend human emotions, Dr Robertson's research is bringing engineers a step closer towards reliable robotic assistants.

Next, we meet Dr Guy Schumann and his team at Remote Sensing Solutions, who have utilised remote sensing technology to develop a user-friendly flood monitoring and prediction system. Such accurate and timely prediction of flood disasters is imperative to give communities and governments time to prepare, and to inform the development of flood defence infrastructure. As extreme weather events are increasing in severity and frequency due to climate change, Dr Schumann's technology could save countless lives across the globe.

As climate change accelerates, the push to obtain 100% of our energy from renewable sources is now more urgent than ever before. So far, efforts to realise this goal have been dominated by installing wind turbines and solar panels. However, because of their intermittent nature, these technologies won't be able to bring about a completely carbon-neutral society by themselves.

Therefore, Dr Donald Fosnacht at the University of Minnesota is investigating biomass as an alternative energy source for when wind and solar power cannot meet demands. His team is

developing new ways to convert raw biomass into biofuels that can be used in conventional coal-based power plants – eliminating the need for the construction of new biomass-burning power plants.

Dr Fosnacht is now hoping to offer his technology to riverside communities in Senegal and Mauritania, where an invasive weed called *Typha Australis* could be harvested as an abundant source of biomass. He proposes that such a project would not only provide an easy way to dispose of the weed on large scales, but it could also provide a carbon-neutral power source to the region.

Our final article of this section showcases another sustainable technology for converting raw material into useful products. Here, we meet Andrew LaTour and his colleagues at MolyWorks Materials, who are developing the 'Mobile Foundry' – a device capable of recycling scrap metal into powders, and at the exact locations where they are needed. The team's efficient metal recycling technology may represent a significant step towards achieving a circular economy in metal manufacturing.

PROGENY: DEVELOPING SAFEGUARDS AGAINST GPS OUTAGES

Global Navigation Satellite Systems such as GPS are the backbone of many global communications, but they are not immune to failure. Progeny Systems Corporation is dedicated to mitigating such disasters if and when satellite-based communications fail, by developing Earth-based systems that work in comparable ways to synchronised satellite networks. As an alternative to GPS, the company's technology could provide communicating parties with a crucial yet inexpensive safeguard against future failures.

Global Navigation Satellite Systems

In today's technological landscape, our society is now more connected than at any point in history. Many of the infrastructures we have come to depend on are themselves dependent on almost instant communications between devices, which are often part of networks spanning many continents. Such vast, intricate networks are made possible by Global Navigation Satellite Systems (GNSSs) – groups of satellites orbiting far above the Earth, which are in constant communication with each other and devices on Earth.

'The GNSS service is adopted worldwide, and its use within a wide range of technology is ubiquitous,' explains John MacKay, a Chief Engineer at Progeny Systems Corporation. 'Not a single cell phone or cell tower, power station, auto and marine navigation, or reference clock operates without some traceable tie to a GNSS constellation.'

The key to the success of this technology is the atomic clocks built into each satellite, which keep time to incredibly high degrees of accuracy.

This allows the GPS receivers to perform a technique named 'trilateration', which involves measuring the time taken for light-speed signals to travel from the satellites to the receivers. Receivers, including cell phones, know the predicted location of each satellite by downloading a file called the 'ephemeris' during the process of receiving the GPS data. From the trilateration measurements, and the known position of all satellites at the time of the measurement, the receivers can continually calculate their positions relative to the satellites and can map this location on the Earth.

'In addition to providing location, the service performs time transfer, whereby any local, low-cost clock can receive time from the service, synchronise to it, and achieve accuracy that is on par with the best clocks in the world,' MacKay continues. 'This enables time accuracy on cell phones to be substantially better than a second.' Most of the time, GNSS systems work so flawlessly that most of us forget that they are even there. However, this stability cannot always be guaranteed.



A Fragile Dependence

Despite their enormous capabilities, GNSS systems are not invincible. For reasons ranging from technological failure to attacks by malicious groups, these systems can fail, and indeed have done so in the past. 'For the world's dependence upon this service, its fragility is deeply troubling,' says MacKay. 'The more amazing aspect of the GNSS than its utility is the impact of its loss. In July 2019, for example, the European GNSS service, Galileo, suffered a signal outage. If this occurred in the US's GNSS system, GPS, the costs incurred by navigation errors and delayed shipments could be upwards of \$1 billion per day.'

‘We are trying to allow ordinary radios to do the same thing as GPS does. Our goal is to make communication systems used in everyday life that perform with a knowledge of time. When we know the precise time that events occur, we can use this information to relate events that are at great distances, and do it much more simply.’



One of the biggest problems with these systems stems from one of their main advantages: due to their pinpoint instrumental accuracy, they can communicate with each other using extremely weak signals. In addition, GNSS systems are so easy to use that it is relatively simple for anyone on Earth to find out how they operate, the frequencies at which they transmit their signals, and calculate their exact positions, leaving them vulnerable to attack.

‘There are several ways that GNSS can be compromised, some of which are malicious,’ explains MacKay. ‘The task is relatively simple to perform; the GNSS signals are extremely low power, and the transmission frequencies well known.’ As globalised infrastructures rely more and more on the accuracy of these position and time measurements, the stakes of failure of GNSS systems are now becoming increasingly apparent. This creates a critical need for users of communications systems to access reliable backup systems, if and when GNSS satellites fail.

Developing a Backup System

To implement these backup systems, the Progeny team, which also includes Senior Electrical Engineer Gregory Hall, and Senior Engineering Manager Ron Murdock, aims to construct infrastructures on Earth that are comparable to those of GNSS systems. ‘In this project, we are trying to allow ordinary radios to do the same thing GPS does,’ MacKay explains. ‘Our goal is to make communication systems used in everyday life that perform with a knowledge of time. When we know the precise time that events occur, we can use this information to relate events that are at great distances, and do it much more simply.’

To do this, Progeny is developing radio hardware that can communicate with nearby radio ‘anchors’ instead of satellites. Including structures such as radio towers, these anchors allow for a bi-directional flow of information. This means that they not only transmit signals, but they can also receive information from distant devices, which can include further instructions about what to transmit. Furthermore, these anchors may themselves be in contact

with timekeeping ‘master’ towers with their own atomic clocks, allowing each anchor to keep its own highly accurate time.

Within these existing infrastructures, Progeny’s mobile radio device can send out a signal to an anchor, asking it to transmit information detailing its position. In addition, the precise time kept by the anchor will allow it to tell how far away it is from the device. If a device is within range of at least three of these synchronised anchors, therefore, trilateration can be used to calculate its exact position, with undiminished accuracy compared with GPS.

‘If GPS is not available, we can provide the same position service with common, low-cost radios, such as cell phones and Wi-Fi hotspots,’ continues MacKay. ‘At a program level, we are making systems that can take this timing information from any radio, and combine it, so that we can take advantage of any transmission, especially if some are better than others, based on location.’ In this system, therefore, the tasks of all components of a GNSS system are carried out by Earth-based counterparts, at very little cost to the user.



Attainable Alternatives to GPS

In their research, MacKay, Hall, Murdock and their colleagues at Progeny have now successfully demonstrated a reliable, Earth-based alternative to GPS in two different ways. 'First, we made radio hardware used for industrial, scientific, and medical data links become "time aware", so that we include the time that data is sent or received in the data stream,' describes MacKay. This insight revealed that devices in practical communications systems can indeed remain in sync with each other during their operations.

In addition, the company's researchers have shown that two radio devices in contact with each other can be made to synchronise their readings for position and time, with undiminished accuracy compared with GPS. 'We worked with a commercial vendor that makes radios to include our "time aware" function in their radios, so that a rugged commercial handheld two-way radio became "time aware",' MacKay continues. 'We tested this radio in a realistic scenario – a plane on one side of the link and a person on the ground on the other, and showed that we operated the same as a GPS radio, with the same position accuracy.'

Achieving these capabilities with such simple technology now represents a significant step towards reliable backup communications systems. Crucially, the hardware would be attainable for virtually any communicating party at very little cost – ultimately ensuring that GNSS outages will become far less of a setback to society as a whole.

Safeguarding Against Future Outages

The Progeny team believes that their technology could become a vital component of many communications systems in the future, for ensuring that their operations don't shut down during GNSS failures. 'This system has universal use, particularly in civil applications,' MacKay explains. 'Critical infrastructure affected by the Galileo outage can be maintained by a mesh of radio links that are time-aware, and transfer time from a known good source. Just as important, it can be deployed quickly, so for emergent outages it can prevent loss of the services needed for infrastructure. It can be suspended just as quickly when normal service is restored. Universal adoption of the technology into cell phones and wifi networks could provide a reliable backup or replacement for GPS.'

Furthermore, the technology developed by the Progeny team could provide a useful basis for communications in built-up areas, where GNSSs can struggle to keep in contact with many closely packed devices at the same time. Since radio communications can take place across many different channels, each with its own unique frequency, this problem could be minimised. 'GPS gets confused in cities due to the signal being blocked by skyscrapers, but Wi-Fi and cell phone signals are usually reliable,' says MacKay.

By implementing such reliable communications systems with a device as common and simple as a radio, virtually any communicating party on Earth can continue its operations as normal during an outage. As the world becomes increasingly connected, the damage that could be unleashed during attacks and outages will only increase. However, Progeny's hardware will ensure that the intricate connections that keep society ticking can remain in place, even during prolonged failures of satellite networks.



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John MacKay has a BSEE degree from the University of Rochester and over 32 years of engineering experience, with a focus on system engineering of hardware intensive systems. He has extensive experience leading multi-disciplinary teams to design, produce, integrate and manufacture complex hardware and software-intensive electronic, sensor and weapon systems. Mackay has also devoted significant effort in the development and advancement of precision time transfer, and its use as a solution for real-world challenges.

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Gregory Hall graduated with a BS in Electrical Engineering from Pennsylvania State University in 1998. He also graduated with honours in Electrical and Computer Engineering from Johns Hopkins University in 2007. His work at Progeny Systems includes the primary radio-frequency and hardware engineering involved with NASA's 'Lunar Surface Navigation Precision Time Protocol Based Trilateration for Planetary Navigation'. In addition, Hall has been the principle investigator for two projects aiming to further develop scalable Ka/Ku band antenna for aerospace applications.

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Ron Murdock has a BSEE degree from the University of Vermont and a 37-year background in the development, testing and evaluation of complex tactical systems, particularly submarine combat systems. Currently, he is a senior engineering manager at Progeny Systems Corporation, where he has been employed since 1998. His technical leadership roles have included systems engineering for advanced submarine control, tactical sonars, sonar signal processing, torpedo countermeasure design, embedded digital data collection systems, sensor manufacturing, acoustic testing and navigation in GPS denied environments.

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FUNDING

IRAD
NASA
NAVAIR
USAF
Office of Naval Research



CART: POINTING THE WAY TO RELIABLE ROBOTIC ASSISTANTS

Robots that assist us with both everyday and highly specialised tasks are no new concept, but so far, their actual development has appeared to be far from becoming a reality. Yet through the research of **Dr Paul Robertson**, Chief Scientist at Dynamic Object Language Labs (DOLL) in Massachusetts, such sophisticated technology is now looking increasingly feasible. By considering how robots can be programmed to recognise tasks and comprehend human emotions, his research could be bringing engineers a step closer towards reliable robotic assistants.

How to be a Good Assistant

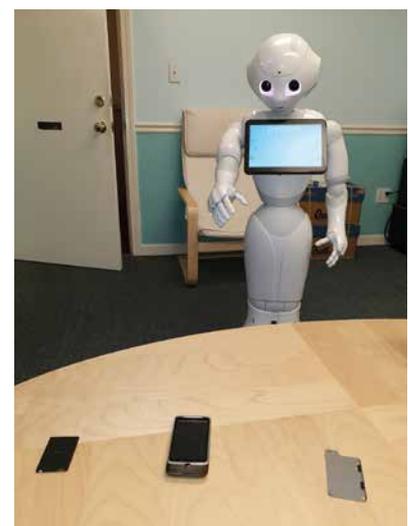
The idea of robotic assistants has existed in the public consciousness for quite some time. These smart machines are often viewed as a highly desirable concept, but until now, they have mostly been confined to the realms of science fiction. Recent advances in the technology, including Amazon's Alexa and Google Home, are perhaps the closest we have come so far. However, if truly reliable robotic assistants are to be fully realised, there are still several fundamental barriers to overcome.

Currently, technologies are limited in their capabilities, since programs lack a basic understanding of how humans think and behave. To offer assistance, they must either only carry out useful tasks when specifically asked, or offer help even when it is not needed, meaning they become invasive to everyday life. In addition, they can only be programmed to carry out very specific tasks; as such, the time required to obtain their assistance can be longer than the time they save. Clearly, the technology needs a new approach.

In his research, Dr Robertson and his team, building on earlier research in story understanding by team member Professor Patrick Winston, have drawn out a set of requirements for building truly useful robotic assistants, which incorporates models of what its users believe and think. If fully realised, the robots would be able to understand what a user is doing and why, recognise tasks they are struggling with, and offer them advice; though only when it is needed. Dr Robertson believes that such 'Theory of Mind' capabilities would allow for significant advances towards genuinely useful robotic assistants. The goal is achievable, but incorporating such human concepts of common sense into a machine is no easy task.

Aiding Repair Missions

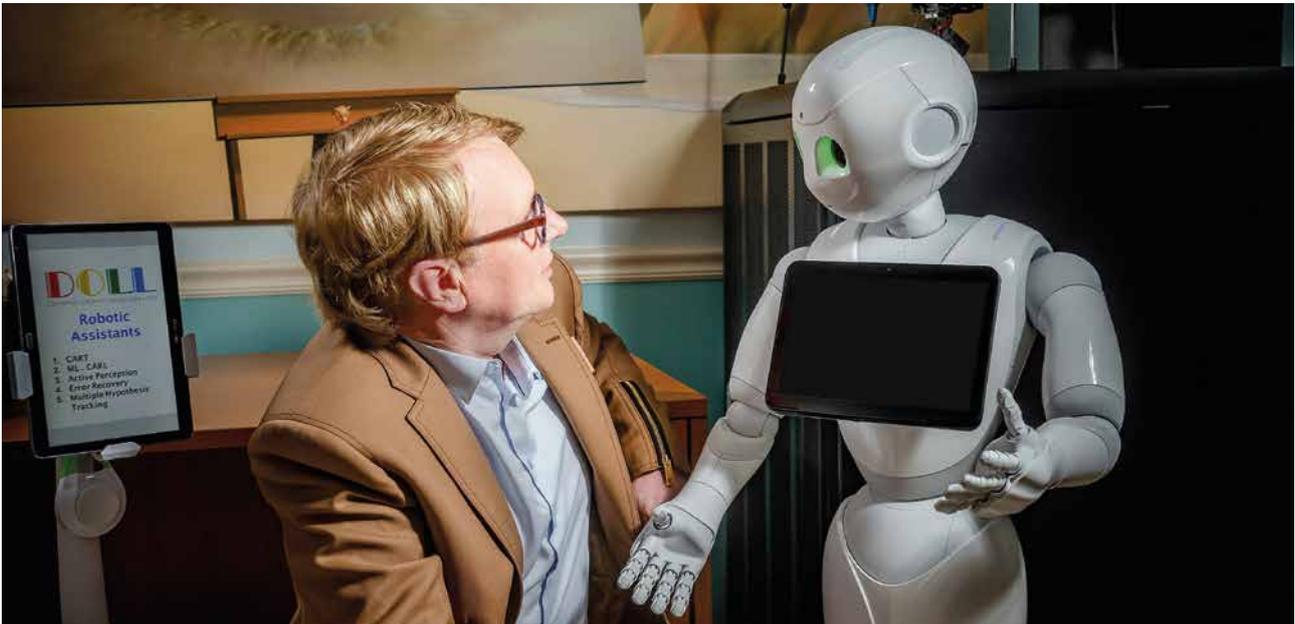
As an initial demonstration scenario, and to avoid short-term limitations of robot dexterity, Dr Robertson has turned his attention towards robots specifically designed to aid repair missions. Such cases are clear examples of where a detailed knowledge of the tasks involved, and a recognition of human abilities, is particularly critical.



To realise these characteristics, Dr Robertson has developed a program named 'Context-driven Active-sensing for Repair Tasks' (CART). 'The idea is simple,' he explains. 'How can a program reflect upon what it is trying to do, and the environment in which it is trying to do it, and to modify itself so as to be more effective? For me, that is the essence of what we call intelligent behaviour.'

Since CART's initial development, Dr Robertson has made meaningful

‘Simply put, we want the robot to reflect on the mission at hand and the human that it must work with, in order to adapt to the specific situation. Then, it can be a good team member in bringing whatever competence it may have to bear on the problem at hand.’



advancements towards developing robots that provide critical assistance during repair missions. ‘Today I am applying these ideas in the context of social robotics, of which the CART project is an example,’ he continues. ‘Simply put, we want the robot to reflect on the mission at hand and the human that it must work with, in order to adapt to the specific situation. Then, it can be a good team member in bringing whatever competence it may have to bear on the problem at hand.’

Therefore, by incorporating the principles of a Theory of Mind, robots programmed with CART can read repair manuals, recognise the different parts they depict, and build a ‘story’ of how they need to be pieced together to achieve the goals of the repair mission.

Embodying Intelligence

Achieving these capabilities has required Dr Robertson to consider a variety of key attributes of reliable robotic assistants. These include the ability of the machines to manoeuvre themselves to get a good vantage point of the repair operation, to understand

what the repairer is doing, and to offer useful guidance in response to the person’s questions. In addition, the robot must use its own initiative to intervene with guidance if the story wanders off track, or if the conditions of the surrounding environment change. As it monitors all aspects of the mission, the robot presently assists the person both through verbal guidance and using physical gestures, but in the future it will participate physically as an able human assistant would.

One particularly important aspect which governs the effectiveness of these attributes is the ability of the robot to understand human emotions. Dr Robertson is achieving this through a modification to CART, named ‘Continuous Affective Robot Learning’ (CARL). This program integrates a ‘fear and reward’ system into CART, which causes robots to develop a ‘desire’ to see a story unfold in a certain way. CARL then ‘fears’ any mishaps, and losing sight of the objective, especially if such events have happened in the past. Therefore, the program can learn to follow prior sequences in which its fears were mostly avoided. If this happens,

the robot will feel a sense of ‘reward’, and so its desire to follow that path again in the future will increase. By desiring certain outcomes, therefore, CARL will react more effectively when potential setbacks arise. This addition of a simple model of emotions allows the robot to improve over time by collecting data about events whose importance is suggested by their affective import. This data is later used to improve future performance through reinforcement learning techniques.

Handling Distractions

In real-world situations, robotic assistants may likely be required to operate in environments presenting many distractions, which could prevent the machines from focusing on a user. Dr Robertson has considered this issue as well: through the integration of a ‘model of attention’ into CART. This model can transform noisy information into stable representations of the story by first acknowledging all objects the robot detects. It can then identify the specific objects that appear in the repair manual.



Thanks to the model, objects are robustly tracked if they appear in an upcoming part of the story, which elevates the levels of attention they receive. In contrast, objects that have already been used, and do not appear again in the story, can be completely forgotten. Through its knowledge of the story, CART can recall what is supposed to happen in the future, allowing its user to focus their attention only on the tasks immediately required of them. The story-driven model of attention results in what we would call common sense behavior on the part of the robot.

Dr Robertson envisages a variety of situations where the use of CART could be particularly critical, including a navy ship under fire, where equipment such as a radar unit has been damaged. Typically, this would require a person to climb up the ship's mast and replace the faulty parts while consulting a repair manual. Clearly, this would be a difficult and stressful task when under fire, making errors likely.

Instead, Dr Robertson proposes that a quadcopter, programmed with CART, would assist the person; hovering behind them as they make the necessary repairs. With its knowledge of the full radar repair process, understanding of the person's capabilities and ability to ignore distractions, the robot would ensure that the person doesn't need to remember everything or continually consult the manual, significantly hastening the repair.

Demonstrating Helpful Gestures

In addition, Dr Robertson has now tested out CART's capabilities in a far simpler, more familiar situation: replacing a cell phone battery. To do this, he has exploited our instinctive reactions to faces and hands gesturing towards objects of interest. These instincts are so strong that we can recognise these gestures even in a simple humanoid robot.

'As humans, as with other mammals, we have become surprisingly accurate at determining what a "face" is looking at,' Dr Robertson explains. 'Humans are extraordinarily good at following gaze and pointing, so it is good to take advantage of this capability.'

Since its initial development, Dr Robertson has made significant strides towards developing robots that provide critical assistance during repair missions. 'CART can point out where the phone is in response to the question "where is the phone";' he continues. 'She always knows where the important pieces are. She can point them out with a combination of head gaze and arm. This combination is very effective. Pointing works very well especially when combined with head gaze.' With this demonstration, Dr Robertson has clearly shown that robots can indeed be genuinely useful in tasks that arise in everyday situations.

Robot Assistants for Everyday Tasks

In the future, Dr Robertson believes that CART will be able to assist humans with increasingly complex tasks, and in increasingly difficult, wide-ranging environments. He also hopes that improvements in robotics, such as the ability to manoeuvre individual fingers, will allow robots to express far more complex emotions and gestures than are currently possible. Ultimately, these advances will make it increasingly easy for human users to respond to and benefit from robotic advice.

Through continuing improvements to CART, Dr Robertson foresees that robots could one day be able to assist with far more diverse types of task than repair missions alone. For now, it seems that the idea of robotic assistants that help us to conduct tasks in our everyday lives seem less far-fetched than ever before.



Meet the researcher

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Dr Paul Robertson holds a DPhil from the University of Oxford, for a research project entitled 'A self-adaptive architecture for image understanding'. Since then, he has worked at numerous prestigious institutions and companies, including the University of Massachusetts at Boston, the University of Texas at Dallas, Artelligence Inc, Symbolics Inc, Massachusetts Institute of Technology, and BBN Technologies. He has had a lifelong interest in reflection in intelligent systems, and the role that reflection can play in adapting responses to changes in the environment. A key interest has been advanced planning, especially in the context of self-adaptation. Today, Dr Robertson's research at Dynamic Object Language Labs (DOLL) Inc centres around the role of emotions and self-awareness in robotic systems as a natural extension from his earlier work on reflection and self-adaptation.

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FUNDING

This material is based upon work supported by the Defense Advanced Research Projects Agency (DARPA) under Contract No. D16PC00144.

FLOOD PREDICTION USING REMOTE SENSING TECHNOLOGY

Floods devastate communities across the globe. A single flood disaster can cause the loss of thousands of lives, and the displacement of millions of people. The devastating effect is exacerbated by the difficulty in monitoring floods and evaluating the information to make the best responsive decisions. To help communities and emergency response teams better predict and prepare for flooding events, **Dr Guy J-P Schumann** and his team at Remote Sensing Solutions in collaboration with the Dartmouth Flood Observatory (DFO) have harnessed remote sensing technology to develop an advanced user-friendly universal flood monitoring and prediction system.

Monitoring Flooding Disasters

Floods are among the most devastating natural disasters on Earth. A single disastrous flood has the potential to displace millions of people from their homes and businesses, cause thousands of deaths, and result in billions of dollars in damages. Floods have affected more people in the 21st century than any other type of disaster. With climate change altering weather patterns and Earth's water cycle, flooding is likely to increase in both frequency and intensity in vulnerable areas.

'Hurricanes and tropical storms in recent years have been particularly devastating globally, with rainfall and inundation footprints far exceeding records and also national response capabilities,' explains Dr Guy Schumann, Principal Scientist at Remote Sensing Solutions, Inc, in Massachusetts.

Accurate and timely prediction of flood disasters is imperative to give

communities and governments time to prepare, and to inform the development of flood defence infrastructure. For predictions to be useful, they need to include probabilities of the likelihood, frequency and the extent of the area that will be affected by flooding events. However, the complex factors influencing flooding events and the scales across which they occur mean that accurate predictions are difficult to achieve.

One of the key requirements for an effective prediction system for flooding is the historical and ongoing monitoring of flooding events. However, the spatial scales at which flooding occurs are often beyond the capacity of regional flood monitoring schemes, so remote sensing – using highly advanced sensors attached to satellites – is a promising solution to gathering the information necessary for future flood predictions.

Remote sensing technology has been in use to monitor flooding since the 1970s, and has improved dramatically



in the last two decades. With the technology now readily available and in use, Dr Schumann and his colleagues at Remote Sensing Solutions and Dartmouth Flood Observatory (DFO), are integrating historical flood records and current flood monitoring, with the aim of creating an accurate and reliable flood prediction system.

In addition, Dr Schumann and his colleagues are creating a user-friendly interface that allows their flood monitoring system to be used by a wide range of organisations and individuals, including disaster response teams, humanitarian aid organisations, insurance companies, and individuals living and working in areas at risk of flooding.

‘Disaster response managers and field operations analysts are often faced with either too much or too little information and with hardly any guidance on how to make decisions based on the data provided.’



New Remote Sensors and Flooding Data

Predicting which areas are at greatest risk of flooding, and when these disasters might occur, requires detailed records of previous floods – including the frequency and timing of the flooding, the depth of the flood waters and the scales across which these events occur, both spatially and temporally. ‘The position of the maximum flood shoreline is the main variable to determine the extent of flood hazard,’ says Dr Schumann.

Sensors capable of monitoring floods remotely have been included in the technology onboard satellites with increasing regularity over the past four decades. Such sensors allow monitoring across greater spatial and temporal scales than was previously possible through regional flood monitoring schemes.

Earlier sensor technologies – optical sensors – had a limited ability to monitor floods consistently throughout the period of flooding, because of their inability to ‘see’ through obstacles such

as cloud cover or dense vegetation. As many floods happen during periods of extensive cloud cover, this meant that there were significant gaps in the data. Nevertheless, historic records obtained using this early remote sensing technology provides a valuable basis for long-range forecasts and allows changes in flooding frequency to be investigated across timescales of decades.

Newer sensors use radar technology that can detect energy similar to that emitted by household microwave ovens. These sensors are not limited by obstacles such as cloud cover, and are capable of producing very high-resolution maps of flooding events throughout the period of the flood.

‘During the last two decades, the amount of satellite missions carrying instruments that can be utilised to map flooding has increased considerably and there is now a general consensus among space agencies and scientists to strengthen the support that satellites can offer for flood monitoring,’ Dr Schumann explains.

With this remote sensing technology

now established and in place, Dr Schumann and his team aim to consolidate previous flood records with powerful predictive models to produce a highly advanced flood prediction and decision support system (DSS) that can be used by any organisation or individual.

Towards a Universal Flooding DSS

The next objective for Dr Schumann and his team is to integrate the remote sensing technology and flooding data into a fully-functioning flood prediction and decision support system (DSS) that can be used in multiple applications, such as coordinating emergency response efforts.

‘Disaster response managers and field operations analysts are often faced with either too much or too little information and with hardly any guidance on how to make decisions based on the data provided,’ says Dr Schumann. ‘There is to date no global decision support system for flood disasters that ingests all the data from existing systems and provides real-time critical information that can guide operational reactions on the ground.’



Dr Schumann and his colleagues aim to combine all the available data in an intelligent way in order to unlock the full potential of these technologies within a flood DSS. The information provided to end-users of the team's flood prediction program – which will be extended from a web-based system to the development of an accessible mobile application – will include details on accuracy, spatial and temporal scales, and uncertainty. This is now already freely available as a first release for [IOS](#) and [Android](#).

Uncertainty in predicting any natural event is an inescapable fact of even the most powerful predictive tools. However, providing levels of certainty along with predictions allows end-users to make informed decisions based on threshold levels of acceptable risk.

'While there may indeed be several good and justifiable reasons for ignoring uncertainties, providing elements of product accuracy is a high priority for organisations and people utilising such products,' says Dr Schumann. His team plans to systematically test and assess the uncertainty of the remote sensors and the flood DSS through extensive comparison to previous flood records.

Meeting the Needs of End-Users

In collaboration with DFO, the team at Remote Sensing Solutions is continuing to refine and build upon their flood DSS, both online and in an application compatible with mobile phones. 'The main challenge lies in maintaining adequate targeted application readiness levels and high interoperability of products and services being delivered,' says Dr Schumann. 'Because capabilities evolve over time, any such interoperable system must be able to easily incorporate changes and improvements.'



Dr Schumann and his team have identified the key tools currently used by flood disaster response organisations to support their decision making, and the capabilities they would like to see available in a flood DSS. They aim to incorporate all of the requirements identified, ensuring users as diverse as the general public, emergency response teams, government departments and insurers are able to access and understand the information provided by the flood DSS.

Additionally, options to customise and interact with the information presented within the maps will give end-users the control and flexibility to filter the results based on their specific needs. For users requiring the capability to analyse flood data, the team's DSS is also compatible with a range of other software. As this system monitors surface water conditions, the flood DSS could potentially provide the advanced monitoring technology to other areas of scientific research. It may be beneficial to monitoring water reservoir levels, wetland conditions, and has great potential for uses in agriculture and ecosystem monitoring.

The flood DSS app developed by Dr Schumann and his team may be an especially useful advancement for emergency responders that need to work against the clock in extremely dangerous conditions. By ensuring that the app is capable of functioning even when a mobile signal is patchy or unreliable, Dr Schumann hopes that his team's technology will increase the efficiency of emergency response teams, by allowing them to adapt their efforts based on real-time changes in flooding disasters.

Dr Schumann and his team's flood DSS and associated mobile app provides a powerful universal tool for monitoring, responding to, and predicting flooding disasters. With flooding events expected to increase in intensity and frequency in the future, this technology is a vital advancement, providing the right information to facilitate decision making, even when faced with the uncertainty of natural disasters.



Meet the researcher

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Dr Guy Schumann earned both his master's degree in remote sensing and his doctoral degree in geography from the University of Dundee, Scotland. He has since accrued more than a decade of experience in the field of remote sensing data integration with hydrodynamic modelling, and particularly radar remote sensing and its use in flood models. He is currently a Principal Scientist at Remote Sensing Solutions, Inc, where his recent research has focused on large-scale flood inundation modelling and integration with remotely sensed data. Dr Schumann is also the CEO and Principal Scientist at RSS-Hydro in Luxembourg – an accredited Private Research Centre for PhD students and postdoctoral researchers. Dr Schumann consults on a number of additional projects, including Interoperability Program activities of the Open Geospatial Consortium (OGC), and is a Visiting Research Fellow in the School of Geographical Sciences at the University of Bristol, UK, and a research affiliate in the Institute for Arctic and Alpine Research at the University of Colorado, Boulder.

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FUNDING

NASA SBIR

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BRINGING BIOMASS INTO THE RENEWABLE MIX

A completely decarbonised society may now be firmly on the agendas of many businesses and world leaders, but the paths that need to be taken to realise this goal still remain far from clear. **Dr Donald Fosnacht** at the University of Minnesota believes that biomass is currently underappreciated as a way to realise a carbon-neutral society. The techniques his team has developed have already been demonstrated on industrial scales in some cases, and even promise to improve the lives of some communities in the developing world. With further research, Dr Fosnacht hopes that biomass will transform the ways in which our industries and power stations function.

Combatting Climate Change

As the urgency of tackling climate change becomes increasingly apparent, the push to obtain 100% of our energy from renewable sources has gained unstoppable momentum in recent years. So far, efforts to realise this goal have been dominated by instalments of wind turbines and solar panels. In reality, however, these technologies won't be able to bring about a completely decarbonised economy by themselves.

When the wind isn't blowing, or the sun isn't shining, energy must either come out from storage, or from another renewable source entirely. Dr Donald Fosnacht and his colleagues at the University of Minnesota are studying a technology that can essentially do both: the combustion of plants, or 'biomass'.

'Our program is looking at the ability to store energy, and an alternative source of energy when stored energy is expended and the renewable source cannot supply what is needed,' describes Dr Fosnacht. 'To do this, we are examining energy storage options

beyond batteries and by conversion of biomass materials into biofuels that can be used in conventional coal-based power plants.'

Since this method wouldn't require policymakers to significantly change current infrastructures for energy production, it is a highly attractive prospect. Implementing it, however, will still require some significant research.

Difficulties with Biomass

Having been compressed and heated for many millions of years, fossil fuels such as coal, crude oil and natural gas are incredibly easy to combust, and release large amounts of energy in the process. Unfortunately, the case isn't the same for newly grown plants.

'Biomass is not easy to use directly due to several problems: logistics are often costly, the energy density is low, and the materials are often very difficult to grind and directly use in current fuel systems,' Dr Fosnacht explains. If plants are not processed in the right way, their use in facilities such as coal-fired power plants will be highly inefficient, and may even cause damage to the facilities.

Therefore, if biomass is to realistically become as important as wind and solar in the renewable energy mix, the techniques used to produce it need to improve. Dr Fosnacht and his team believe that by developing better ways to convert plants into energy-dense, easily combustible fuels, this conversion will begin to look far more realistic. They envisage a wide variety of applications of such a fuel, including carbon-neutral industrial processes, distributed power generation, conversion into charcoal substitutes, and the development of even more advanced products such as liquid fuels.

New Processing Technologies

To achieve these capabilities, Dr Fosnacht describes two techniques for implementing the process of 'torrefaction', in which biofuels are roasted at low temperatures to produce dry, energy dense and easily combustible char. The first of these is an 'indirectly heated rotary kiln' – a slowly rotating tilted cylinder in which raw biomass is fed in at the top end, and is heated by external means to drive out volatile matter and increase its fixed carbon content as it passes

‘Our laboratory philosophy is to help take ideas whether generated in our own laboratory or from a collaborator and show what can be practically achieved.’



Biomass in Industry

Currently, powdered coal is an important ingredient in the chemical reactions that convert iron ore extracted from mines into pure metallic iron, for use in steelmaking. Yet through several studies, Dr Fasnacht and his colleagues have shown that the biofuels produced with their technologies can perform exactly the same function, while still being a reliable fuel source.

‘We have participated in various trials at both industrial applications such as power generation and steelmaking,’ Dr Fasnacht recounts. ‘They show that the converted biomass materials can be a good substitute for coal. In addition, we have tested the produced fuels on stationary hearths using mobile steam boilers, and found that it can completely displace coal.’

Furthermore, the researchers believe that through further development of their biomass conversion techniques, a variety of other more valuable products could also be produced. ‘These include chars for agricultural use, and the production of clean water through

through the structure. Once it reaches the bottom, the material will have transformed into a charcoal-like substance. Secondly, a ‘moving bed reactor’ involves processing biomass in a columnar reactor, where biomass and super-heated steam flow together through the reactor and the biomass is again transformed into a char material. Dr Fasnacht has demonstrated the feasibility of both reactors at his facility.

Another technology that Dr Fasnacht is developing is called hydrothermal carbonisation (or ‘wet torrefaction’), in which both pressure and temperature are employed to treat the biomass. ‘This technology allows some ash material to be removed while it concentrates

the carbon and increases the fuel value of the biomass to much higher levels,’ says Dr Fasnacht. ‘We have found that the converted materials can be easily densified using methods including pelleting and briquetting.’

The researchers have now demonstrated these processes on industrial scales at their facilities; producing tons of biofuel on a campaign basis that is compatible with coal-fired power plants. Now, they are considering how their technology could be applied to tasks beyond power generation alone, including industrial processes where fossil fuels are still essential, such as steel production and chemical manufacturing.



absorption of undesired chemical agents onto char surfaces,' describes Dr Fosnacht. In addition, he notes that the char material may be a good carrier for microbial agents that can be used to enhance agricultural performance.

This would be possible since such biofuels have many small pores on their surfaces, increasing their surface area. In turn, this would make them better at trapping the contaminants and impurities present in untreated water. Armed with this combination of demonstrated uses and realistic roadmaps to potential applications, Dr Fosnacht has recently turned his attention to how his team's technologies could help to improve the prospects of poorer communities.

Biomass in Developing Countries

In 2016, Dr Fosnacht travelled to the Senegal River Region in West Africa. In recent years, an aquatic weed named *Typha Australis* has unleashed widespread disruption on activities including agriculture, fishing and access to drinking water along the river. On the trip, Dr Fosnacht met with local researchers and communities to examine the potential of *Typha Australis* as a biofuel. He proposes that such a project would not only provide an easy way to dispose of the weed on large scales, but it could also provide a carbon-neutral power source to the region, where a lack of sufficient infrastructure currently hinders the development of other renewables.

'We have visited both Mauritania and Senegal and found that *Typha Australis* may be suitable feedstock for conversion of fuel products along the Senegal River,' Dr Fosnacht describes. 'By converting the material to a fuel, it potentially could allow

various advantages for the communities along this river, including job creation, improved fishing, elimination of disease vectors, and improved river access.'

Dr Fosnacht's findings from the trip indicate that with the help of the technologies developed in his team's previous research, *Typha Australis* could be rapidly harvested from waterways throughout the Senegal River and converted from a nuisance into an economic resource.

In addition, once it has been converted to char, the large amounts of energy contained in the biofuel can be easily stored for indefinite periods. When required, the fuel could then be immediately used for everyday activities such as cooking, and could also make significant contributions to the electricity supplies of the two nations which straddle the river.

Encouragingly, Dr Fosnacht reported enthusiasm amongst many local people when discussing how his technologies could be built and scaled up in Senegal and Mauritania. He now believes that through further developments, his methods could become hugely beneficial to countries across the developing world, where extensive distribution infrastructures for renewable energy have yet to be built.

Towards Commercialisation

Dr Fosnacht and his colleagues now predict that the capabilities of their techniques could soon stretch even further. Currently, they are studying how effective they could be in realising carbon neutrality in a variety of public services. 'We think our technologies may find practical use in processing municipal solid waste, plastics and other materials,' Dr Fosnacht summarises.

Furthermore, the scale of the conversion processes they have already achieved provide the team with reliable pathways towards the implementation of biofuel conversion technologies on commercial scales.

As Dr Fosnacht concludes, 'our laboratory philosophy is to help take ideas whether generated in our own laboratory or from a collaborator and show what can be practically achieved.' With such collaborators in environmentally conscious industries and the developing world, where a widespread enthusiasm for tackling climate change has taken hold, this mindset promises to inspire a real force for change.

Overall, the insights gathered by Dr Fosnacht and his team have the potential to provide a significant boost to the immense efforts required globally to obtain 100% of our energy from renewable sources. If the energy that is naturally cycled through Earth's ecosystems can be utilised on global scales, instead of that locked deep underground for many millions of years, we may be one step closer to our goal of true carbon neutrality.



Meet the researcher

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Dr Fosnacht received his PhD in metallurgical engineering from Missouri Science and Technical University in 1978. After initially working in the steel industry, and in consulting, he joined the University of Minnesota Duluth's Natural Resources Research Institute as Director of the Center for Applied Research and Technology Development. He currently is Associate Director of the Institute. He has served on various state task forces related to minerals or energy with industrial, small business, governmental and academic collaborators. He has directed work related to iron ore conversion to metallic iron, renewable energy, and examining the efficacy of both torrefaction and hydrothermal carbonisation in pre-treating biomass to create enhanced energy fuel products.

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Minnesota Power
Oregon Torrefaction
New Biomass Energy
Airex
Biopower Sustainable Energy
Terramax
Permanente

FUNDING

US Commerce Department, Economic Development Administration
US Department of Energy
US Endowment for Forestry and Communities
US Department of Agriculture – US Forest Service
Minnesota Department of Commerce
Xcel Energy Renewable Development Fund
Permanent University Trust Fund – University of Minnesota
Initiative for Renewable Energy and the Environment – University of Minnesota
Private Industry

UMD

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Driven to Discover

CREATING A CIRCULAR ECONOMY FOR SUSTAINABLE METAL MANUFACTURING

Facilities for recycling metal parts at the locations they are required would be a major milestone in the global struggle towards sustainable industry. Yet for all its advantages, the innovations required to realise such a goal are a daunting prospect. Now, **Andrew LaTour** and his colleagues at MolyWorks Materials are bringing the idea one step closer to reality, through the development of their 'Mobile Foundry'. The company's work could soon provide a new basis for developing a completely closed-loop economy in areas related to metal manufacturing, potentially slashing the industry's negative environmental impacts.

Metal Recycling

Recently, research into manufacturing techniques has revealed significant advantages of converting metal parts into fine powders when they are scrapped. From these powders, new metal parts can be manufactured from scratch through the use of 3D printers, bypassing the need for purchasing new parts. Ultimately, this could create a closed-loop life cycle for such parts, avoiding the necessity for further materials to be extracted from the Earth. Such a system would not only save money, but would also reduce the ecological destruction and emissions associated with mining.

One of the most basic principles of economics is known as 'economies of scale' – the idea that any upscaling in the production of a product will directly correspond to lower production costs. The principle means that in order for such a recycling system to be lucrative, vast amounts of materials need to

be manufactured in just a few major, centralised facilities, before being shipped locally. In this case, bulk metals would be gathered by recycling facilities, and then shipped to centralised powder producers. Afterwards, they would be 3D printed into new parts before being shipped back to the original depot.

Despite the economic track record of this system, Andrew LaTour and his colleagues at MolyWorks Materials believe that it has major shortcomings: the shipping of materials over large distances incurs high fuel costs, requires time-consuming logistics, and the emissions significantly contribute to climate change. Metal powders in particular are extremely heavy, which exacerbates the problem further. Because of these deep-rooted issues, the team at MolyWorks now envisages an overhaul of the techniques used to recycle metals worldwide.



Advantages of Distributed Recycling

As mining operations wind down worldwide, incentives are growing for manufacturers to develop smaller, more distributed facilities for producing metal powders. In a recent manuscript, LaTour acknowledges numerous advantages of such systems. He proposes that if metal parts can be scrapped, turned into powder, and 3D printed all at the same depot, huge amounts of wasted energy consumption could be removed from the equation, and tedious shipping regulations could be avoided.



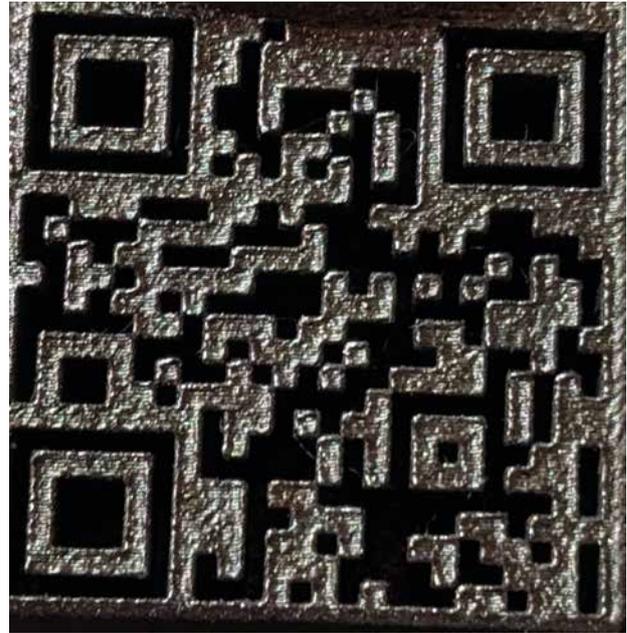
Proof-of-concept testing revealed that where comparable operations in today's economy typically take weeks to months to complete, they could be finished in just days to weeks in an overhauled system – slashing wasted time by up to 90%. In addition, the amount of materials and fuel consumed during the procedure could be reduced by as much as 95%. If realised, such a system would very clearly be far more economically viable and environmentally friendly than current processes. To achieve it, however, LaTour identifies several barriers that must first be overcome.

Difficulties with Melting and Atomisation

To convert bulky metals into powders, two overall steps are required. First, they must be melted; and then, blasted into sprays of fine particles in a process named 'atomisation'. Techniques for melting metals have improved significantly in recent years. In the past, it was done inside crucibles coated with materials such as graphite or ceramic to prevent contamination by impurities. However, these coatings are consumed during melting, which makes the process unsustainable and unable to melt metals at the high speeds required for industrial applications.

The more modern 'plasma cold hearth', constructed using highly conductive materials such as copper, can heat up plasma to temperatures as high as 24,000 degrees, inducing far higher melt rates in the metals exposed to the plasma. However, graphite and ceramics still cannot be completely avoided in these devices, and the melting chambers must be physically entered for cleaning, risking the safety of the operators.

Many other factors must also be optimised, including the ideal gas-to-metal ratio, which affects the sizes of powder particles, gas pressure, metal pour rates, and the type of alloy used – all of which raise the complexity of the problem further.



The Mobile Foundry

To address each of these issues, LaTour and his team at MolyWorks recently developed the Mobile Foundry. This device is capable of melting and atomising metals safely and efficiently, and at the exact locations where their powders are needed. To process metals, the device uses a specialised technique for plasma cold hearth heating, followed by atomisation using a high-pressure stream of argon gas to produce a powder composed of mostly spherical particles.

The Mobile Foundry can work with 16 different metal alloys, including titanium, steel, stainless steel, nickel, aluminium, and copper. In the most recent demonstrations of the device's capabilities, LaTour and his colleagues have shown that it can rapidly process metals as large as 15 centimetres in all three dimensions, without the need for any ceramics or graphite, while still minimising the risk of contamination.

Furthermore, the orientation and shape of the atomisation chamber make it less confined for those needing to enter it, making the device far easier and safer to clean.

Plasma-arc Melting

The first upgraded element of the Mobile Foundry was the 'transferred-arc' plasma cold hearth melting system. Typically used to weld metals, plasma arc devices operate by forming powerful arcs of electricity between an electrode, and the metal object being worked on – transferring large amounts of heat in the process. High-temperature plasma is then created as gaseous atoms in the path of the arc are broken down into their constituent nuclei and electrons.



By passing an arc through unreactive gas such as argon, LaTour's team has found that they can easily produce plasma free from any impurities, allowing for highly efficient melting when it comes into contact with metal. They also found that as the metal liquefies, it can be refined through separation into elements with different densities – allowing unwanted, lower-density elements to evaporate away. Since this technique achieves fast melting with relatively little effort, the process can become far more environmentally friendly and economically sustainable than previous crucible-based methods.

Atomising the Stream

Next, LaTour and his colleagues developed a system for 'horizontal free-fall' atomisation, in which a falling stream of molten metal meets a fast, horizontal flow of atomising gas. To do this, they used 3D printing to create a series of intricate nozzles. When gas is passed through them, the nozzles create complex vacuum structures that direct metal streams into the regions where they can be broken up by the horizontal gas flow.

Having demonstrated atomisation for a variety of alloys, the researchers then explored the ways in which the process unfolds by capturing it on a high-speed camera. By capturing as many as 60,000 frames per second, the camera allowed the team to identify the exact mechanisms that cause the stream to thin out and break up, giving rise to diverse particle morphologies in the final powder product. It also enabled them to differentiate between the particles produced in different parts of the stream, whose velocity continually changes as it falls.

At the lower end, where the metal had accelerated to higher speeds, LaTour and his colleagues observed that the atomising gas breaks it up into smaller particles, due to physical processes including 'plume-sheet' and 'sheet-thinning' modes, inducing secondary atomisation. Conversely, larger particles were formed in the lower velocity upper regions of the stream, where 'bag' and 'bag-plume' modes were the more dominant physical mechanisms.

Studying Shapes and Sizes

To analyse the morphologies of the atomised particles in further detail, the researchers employed a technique called scanning electron microscopy, which produces images of material surfaces using focused beams of electrons. They saw that most particles were generally spherical in shape, often appearing with agglomerations of several smaller 'satellites' clustering around them. The shapes and sizes of the particles showed subtle variations when different alloys were used.

In their attempts to quantify them, LaTour's team identified 110 unique configurations overall – each affecting the yield, production rate and efficiency of the atomisation system. In future studies, LaTour and his colleagues now hope to discover new ways to optimise these values, without affecting the quality of the final product. With these advances, MolyWorks' Mobile Foundry is moving closer towards commercial success. Ultimately, this could make localised facilities for scrapping, atomising and manufacturing metal parts a more realistic prospect than ever before.

A Circular Economy

As both the shipping and manufacturing sectors look towards reducing their environmental impacts, the development of the Mobile Foundry comes at a crucial time. The potential for globally distributed metal recycling brought about by MolyWorks may represent a significant step towards achieving a circular economy in metal manufacturing. As the global economy continues to grow unabated, the Mobile Foundry, and technologies like it, could one day prove to secure our futures, without unleashing irreversible damage on the natural world.



Meet the researchers

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Andrew LaTour was awarded his degree in Chemical Engineering from San Jose State University in 2011. He has over 12 years of experience in Research and Development, and is familiar with a wide variety of equipment and processes, through the invention of chemical and material formulations, as well as novel equipment. Most recently, he was the co-founder of MolyWorks Materials Corporation, where he now works as Chief Innovation Officer.

Matthew was awarded his BS degree in Manufacturing Engineering from California State University Chico, in 2001. He now has 15 years of experience in metallurgy R&D. He is an industry expert, having designed, fabricated, developed, and scaled up metallurgical systems. With a little help from Andrew and Chris, Matt built our first mobile foundry prototype in his front yard, utilising his homemade containerised machine shop to craft furnace components.

Christopher Eonta achieved his BS degree in Chemical Engineering from San Jose State University in 2011. He is an accomplished inventor and entrepreneur. With a strong background in chemical engineering and metallurgy, Christopher has invented metallurgical systems and brought together a skilled team of investors and talented individuals at MolyWorks Materials Corporation. Christopher has commercialised products, sold capital equipment internationally, and received strategic investments from two S&P 100 Companies.

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US Patent 62/790,103, Method for Manufacturing Nickel-Based Superalloy Components Using Recycled Feedstock and Additive Manufacturing
US Patent 62/781,107, Method and System for Manufacturing Landing Gear Components Using Additive Manufacturing
US Patent 16,135,191, Deployable Manufacturing Center (DMC) System and Process for Manufacturing Metal Parts



MATERIALS SCIENCE





ACCELERATING TECHNOLOGICAL PROGRESS THROUGH NEW MATERIALS

This section of the edition reports on some exciting developments in materials science – a critical field encompassing the discovery and characterisation of new materials. Over the following pages, we meet several pioneering scientists who are developing new materials for various advanced technologies – from those creating nanoparticles for efficient solar cells, to others inventing organic coatings to protect metal from costly corrosion.

Our first article focuses on thin films – layers of materials that can range from just a fraction of a nanometre to several micrometres thick. Thin films are vital to our modern electronic devices, forming critical components of displays and integrated circuits. The arrangement of atoms within a thin film gives rise to its unique properties, so scientists are eager to find new ways of observing the atomic structure of such films, in order to fine tune their electronic behaviour. Here, we meet Professor Yoshio Waseda at the Institute of Multidisciplinary Research for Advanced Materials in Japan, who has created a new method to study the atomic structures of thin films in great detail.

Next, we meet Dr Ghada Koleilat at Dalhousie University in Canada, and showcase her career of breakthroughs in creating advanced materials for solar photovoltaic technologies. Throughout the last two decades, Dr Koleilat has developed new ways to fabricate and process thin films, nanoparticles and carbon nanotubes towards the production of highly efficient solar cells.

Also developing complex materials for advanced technological applications is Dr Sascha Preu at TU Darmstadt in Germany, who we meet in the third article of this section. Here, we showcase his team's research into a new erbium arsenide-based material, which shows promising behaviour as a photoconductor. Unlike semiconductors, whose electronic properties can be tuned by changing the temperature, a photoconductor's electronic behaviour is influenced by the light it absorbs. Dr Preu's work has greatly improved the prospects for photoconductors in various applications, including spectroscopy, imaging and non-destructive testing.

Next, we focus on the intriguing behaviour of a class of materials named ferromagnets, in which the properties of the constituent atoms allow the material to remain permanently

magnetised. Here, we feature Professor Andrei Pimenov at the Vienna University of Technology, who investigates how particles called 'electromagnons' can cause light to move in mysterious ways within ferromagnets. His team's research could open up new ways to control the propagation of light within these unique materials, with numerous exciting technological applications.

From here, we shift our attention to organic materials, where we introduce Jianguo Wang at AnCatt Inc, a company that has formulated anticorrosion coatings based on a polymer called polyaniline. With metal corrosion estimated to cause \$2.5 trillion USD in annual losses worldwide, Wang's coating technology offers an environmentally sustainable solution to a significant global problem.

Our final article of this section documents an exciting conference, first hosted in September of 2019, which aims to foster collaboration in the blossoming field of nanomaterials research. Spearheaded by Yerevan State University in Armenia, the Advanced Nanomaterials and Methods (ANAM) 2019 International Workshop and Young Scientist School promises to spark further innovation in nanomaterials research in Armenia and the surrounding regions.

UNDERSTANDING THE ATOMIC STRUCTURE OF NEW MATERIALS

Materials science – the discovery and characterisation of new materials – drives forward the creation of new technology. In particular, the development of thin films of materials is vital to the electronics industry, as they are used in various device components such as displays and sensors. The properties of these materials are defined by their atomic structure, and until recently it was a major challenge for scientists to accurately characterise this. Towards this aim, **Professor Yoshio Waseda** and his team at the Institute of Multidisciplinary Research for Advanced Materials have developed a novel method for characterising the atomic structure of thin films.



Materials Science

The material world around us is changing rapidly. The discovery of new materials, or finding new ways to process and use existing materials, is what drives forward the creation of new technologies. From the discovery of metal alloys and rubber in the early 1800s, to the characterisation of graphene in 2004, scientists are discovering new materials all the time.

Materials scientists discover and design new materials that can be used across many different technologies. They hope to understand how the processing of a specific solid material can influence that material's properties through alterations to its atomic structure.

Today's materials research focuses on a wide range of areas, including ceramics, polymers and nanomaterials. The study and development of new materials is particularly important for the field of electronics. Many of our everyday electronic items, such as LCD televisions

and mobile phones owe their evolution to innovative discoveries, including oxide semiconductors, composite plastics and strengthened glass.

For instance, the development of the smartphone as we know it would not have been possible without the invention of the liquid-crystal display and thin-film transistor (TFT). The field effect transistor (FET), a vital component of many computer devices, also comprises a thin-film semiconducting material and requires far less energy to operate than previous transistors, helping to meet society's requirements for energy saving.

The arrangement and types of atoms in a material directly affects the material's behaviour, such as its electronic properties. Therefore, scientists are always eager to find new ways to study atomic structure in detail, so that they can more effectively fine tune material properties. Towards this aim, Professor Yoshio Waseda and his colleagues at the Institute of Multidisciplinary Research for Advanced Materials in Japan have developed a novel method to study the atomic structure of thin films of materials.

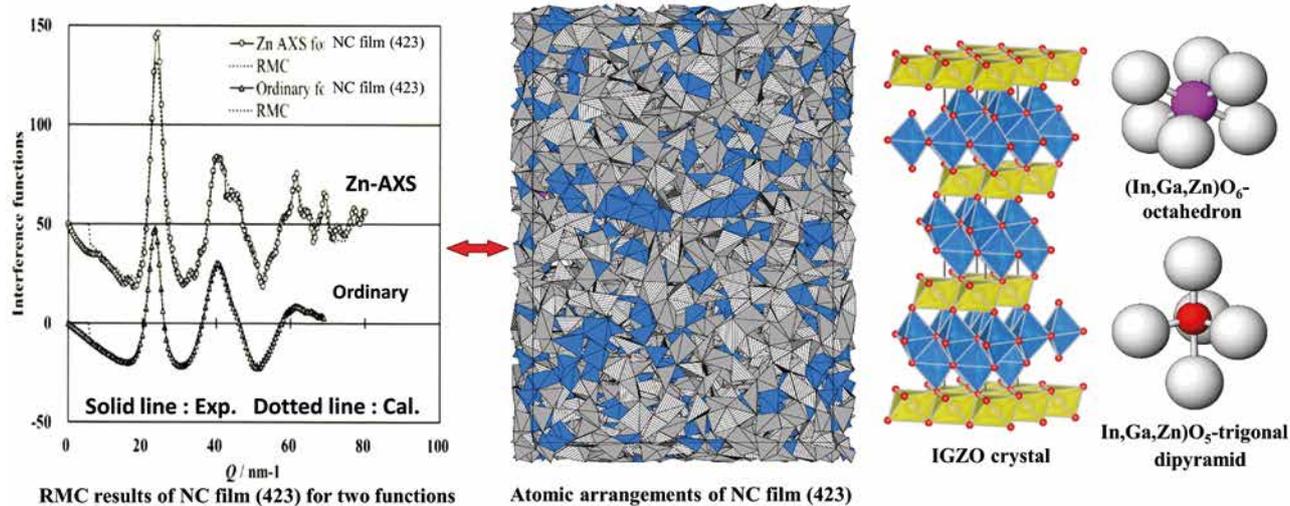


Figure 1. RMC results reproduce two structural functions independently obtained from measurement. Note that 423 is the ratio of In_2O_3 , Ga_2O_3 and ZnO .

Amorphous Materials

Materials are usually made of multiple types of atoms (different elements). By understanding how different combinations of elements create different physical properties, scientists can begin to simulate new materials to meet specific demands.

Scientists study the atomic arrangement by looking at how well ordered the constituent atoms or molecules are in a given material. They look at how regularly spaced neighbouring atoms or molecules are, as well as how random their distribution is across a wider area within a material. In crystalline solid materials, these units are very well ordered. Each atom or molecule has multiple neighbours that are equal distance from each other (an ordered atomic structure).

However, so-called ‘amorphous’ materials have a disordered atomic structure, with no repeating pattern. ‘In liquids and glass,’ describes Professor Waseda, ‘the atoms or molecules are distributed at random with little space between them.’ Professor Waseda’s research focus is to improve our understanding and make it easier to study the atomic structure of amorphous materials, particularly amorphous thin films (layers of material between a nanometre and

several micrometres thick). Thin films often possess unique properties that make them ideal for many device applications, including integrated circuits.

Thin films play a vital role in modern technology that we as consumers often take for granted, which is their role as semiconductors. Semiconductors form the basis of our modern electronic devices, where they perform vital functions. Currently, the most common semiconducting material used in our electronic devices and solar cells is silicon. The ability to measure the atomic structure of alternative types of semiconductors allows material scientists to design new semiconducting materials for specific uses, such as high-performing thin films for next generation electronic devices.

X-Ray Scattering Techniques

Studying the atomic structure of an amorphous material is a challenge, as the atoms or molecules are randomly distributed with no regular, recurring pattern. In order to study the atomic structure of amorphous thin film materials, Professor Waseda and his team combined x-ray scattering techniques with mathematical models.

X-ray scattering is a non-destructive method of analysing a material. When

an x-ray beam hits a sample of material, it is scattered (absorbed and re-emitted in different directions) by individual atoms or molecules in the material. Scientists can study the intensity and patterning to this scatter to determine the atomic structure and other properties of thin films.

The team used a technique called x-ray scattering for obtaining the ‘radial distribution function’ of the material. The radial distribution function describes the probability of finding atoms within a specified volume and within a particular distance of each other. In addition, the local environmental structure around a specific element is required for describing the structure of an amorphous material. For this purpose, the team also employed anomalous x-ray scattering combined with a simulation technique called Reverse Monte Carlo. Anomalous x-ray scattering is known to be useful for both crystalline and non-crystalline materials for studies of surface and bulk materials.

The team’s method has been successfully used to characterise the structures of thin films that are less than a micrometre thick, and can be applied to both crystalline and amorphous materials. This has provided a new in-depth look at the properties of these materials.

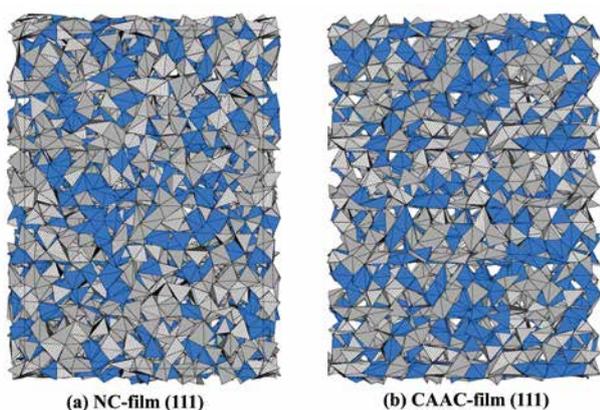


Figure 2. Atomic-scale structural model for reproducing two independent structural functions. Cross-hatched pattern: oxygen-polyhedral units around In; grey: oxygen-polyhedral units around Zn; blue: oxygen-polyhedral units around Ga.

IGZO Films

In their recent work, Professor Waseda and his team have been investigating the structural properties of a particular material called indium gallium zinc oxide (IGZO), which is a semiconducting material. Thin films of IGZO are already in use in a variety of electronic devices. For example, IGZO thin films can be found in flat panel displays, such as smartphone screens and tablet displays, as they have an improved power consumption rate compared to other thin films, providing energy-saving features.

There are multiple types of IGZO film, including a nanocrystalline film and a newly discovered crystalline film (CAAC IGZO film). These both show features that imply their structure includes individual crystals, indicating that there could be some order within their structures. However, scientists had not yet fully elucidated the discrete crystal structures within these films. Professor Waseda and his colleagues have been investigating their structure to better understand their physical and chemical properties.

Using their anomalous x-ray scattering method, the team investigated the 'anomalous dispersion effect' of an element of interest by tuning the incidence x-ray energy to collect data on the atomic structure of that specific element in the thin film. They also combined this data with simulations to create an atomic-scale model for the IGZO films. Their aim was to gain the atomic arrangements in order to independently reproduce two structural functions obtained from measurement (see Fig. 1).

The team initially discovered that there was a distinct crystalline feature within the NC (nanocrystalline) and CAAC films (see Fig. 2). It was previously thought that IGZO films were structured in layers, with slabs of indium and oxygen alternating with slabs of zinc, gallium and oxide molecules. The team found that the four elements are basically mixed together

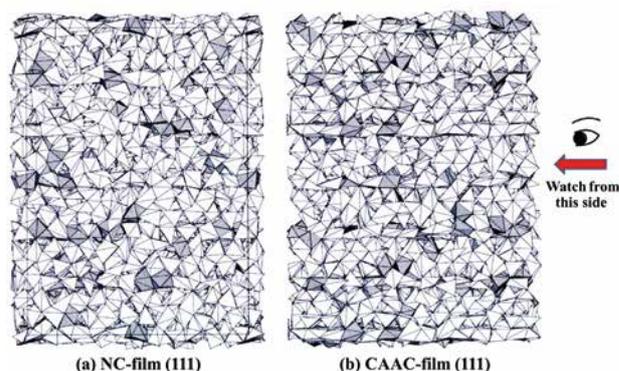


Figure 3. When focusing on the atomic coordination state only using the same model without colour coding, the residual crystalline clusters attributed to the particular layered structure of IGZO are detected in both films, particularly when observed from the side.

to form crystalline clusters in both types of film, each of which exhibits the characteristic layered-structure of IGZO (see Fig. 3).

The team refer to this structure comprising nanometre-sized structural features as a crystalline-cluster-composite (triple C) system. This atomic arrangement of nanometre-sized crystalline clusters contributes to the resilience of this material against atomic rearrangement, even when the structure has a relatively high density. Such features are promising for the production of large square films, while also benefiting the production of IGZO films with sufficient reliability for device fabrication in microelectronics.

The Future of Materials Science

This combination of gathering data from laboratory analysis techniques along with modelling atomic structures is an important aspect of materials science research. Material scientists hope to fully characterise materials that are already in use to understand how their atomic structure relates to their physical properties, such as their ability to conduct electricity or how brittle they are under certain conditions. Once scientists can determine exactly how different chemical combinations produce these properties, they can easily simulate a material with those required properties.

In a world of rapidly developing technology, it is vital we fully understand the properties of new materials to ensure we can get the maximum value from each exciting discovery. Professor Waseda's x-ray scattering technique to accurately model the atomic structure will play a vital role moving forward. As a non-invasive, non-destructive technique that can be applied to a wide variety of material types, it will be invaluable to understanding the chemical, electrical and magnetic properties of both existing and yet-to-be discovered materials.



Meet the researcher

Professor Yoshio Waseda

Emeritus Professor of Tohoku University

Founding Director of the Institute of Multidisciplinary Research

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Professor Yoshio Waseda is a materials scientist based at Tohoku University in Sendai, Japan. He is particularly interested in the structure of non-crystalline materials, and his long research career has led to over 700 publications. After completing his PhD in Materials Science at Tohoku University in 1973, he went on to lecture there, interspersed with some time at the University of Toronto and the University of Pennsylvania. Professor Waseda founded the Institute for Advanced Materials Processing in 1993 and the Institute of Multidisciplinary Research for Advanced Materials in 2001, and is currently Director of the Institute of Electromagnetic Materials. He has been the recipient of many awards such as TMS Leadership award and Honda Memorial Gold Metal award, and was most recently awarded The Order of the Sacred Treasure from the Emperor of Japan. Professor Waseda also holds five patents, and regularly collaborates with industry.

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A CAREER OF BREAKTHROUGHS IN ADVANCED MATERIALS

Solution-processed nanomaterials, such as quantum dots, are some of the most exciting and widely studied materials in nanotechnology today, but reaching this point has been no easy task for scientists. From the very start of her career, **Dr Ghada Koleilat**, now an Assistant Professor at Dalhousie University in Canada, has been a renowned pioneer in this field – devising innovative new solutions to some of nanotechnology’s most pressing questions. Her numerous breakthroughs have brought about some profound new ways of thinking in one of the most rapidly developing energy generation technologies in the modern world: solar cells. Their findings may help to improve the performance of quantum heat engines.

Quantum Dots

Some of the most ubiquitous elements of today’s technological devices are materials named semiconductors, whose conductive properties fall in between those of conductors and insulators. In recent years, researchers worldwide have aimed to push the capabilities of these materials ever higher.

To date, one of their most cutting-edge developments are semiconductors scaled down to just a few atoms across – so small that the intriguing effects of quantum mechanics become relevant in governing their behaviours. Known as ‘quantum dots’, these nanoscale semiconductors, whose behaviours strongly mimic those of individual atoms, are now widely studied in the field of nanotechnology, particularly relating to how they interact with light.

When illuminated by ultraviolet light, one of the electrons in a quantum dot

will jump from its insulating, or ‘valence’ band, into its conducting band. As it jumps back to the valence band, this electron will then emit a particle of light – a photon – whose colour directly depends on the difference in energy between the two bands.

Yet despite the numerous advantages of this property, many challenges remain before quantum dots can be fully exploited. For instance, when they are exposed to air, today’s quantum dots will typically break down within just a few minutes, significantly limiting their prospects for use in modern technologies.

Redesigning Production

Straight after finishing her undergraduate degree in electrical engineering, Dr Ghada Koleilat committed her research to tackling this challenge head-on. Through a graduate project at the University of Toronto, she did this by exploring the



chemical processes that unfold as quantum dots are produced. Through her results, published in the journal *ACS Nano* in 2008, she proposed that the inconveniently short lifetimes of quantum dots stem from the use of organic molecules named ligands in their production process. These ligands bind to a central metal atom, and allow quantum dots to become evenly dispersed throughout a mixture.

Dr Koleilat needed to devise an entirely new way to process quantum dots from scratch. After becoming well acquainted with a wide array of manufacturing techniques, she succeeded in designing and creating quantum dots with far



longer lifespans than had ever been achieved previously – while maintaining their even dispersion.

This technology has been licenced to the semiconductor production company, InVisage Technologies, now owned by Apple. Dr Koleilat's advanced quantum dots are now the core of the manufacturing techniques used by the company and will soon provide a basis for a new range of phone cameras, set to enter production in the near future.

Pushing the Limits of Solar Cells

Today, perhaps the most widely explored application of quantum dots are solar cells – one of the most promising and rapidly evolving forms of renewable energy currently available. Typically, solar cells operate using the photovoltaic effect, in which photons of sunlight excite the electrons in semiconductor materials to the conducting band, where they can move freely. Once in the conduction band, these electrons can travel around a circuit towards a positively charged part of the cell, creating a flow of electricity that can be harvested.

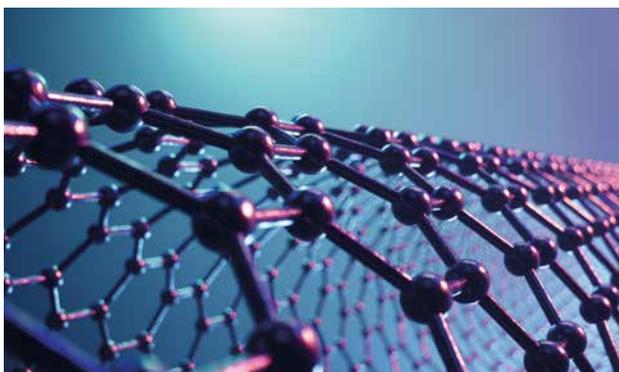
Today, conventional solar cells require semiconductor materials that contain just the right mixtures of impurities to output as much electricity as possible. Yet through her research, Dr Koleilat shows that materials hosting evenly dispersed mixtures of quantum dots could be better suited to this task. Since the gaps between the conducting and valence bands in quantum dots are easily tuneable in the manufacturing process, they are ideal for efficiently generating electricity from sunlight. To ensure optimal performance, however, their compositions must be meticulously engineered.

Integrated Quantum Dots

Following her initial work with quantum dots, Dr Koleilat embarked on her PhD project, in which she explored the possibility of a wider usage of quantum dots in solar cell manufacture. Funded by Canada's Natural Sciences and Engineering Research Council (NSERC), she developed and patented the world's first solar cell in which materials containing long-lived, evenly-suspended quantum dots were used in conjunction with other semiconductor

materials. Through collaboration with industries including Oerlikon Solar, she was able to integrate her quantum dots into existing silicon-based technologies, providing the ideal platform for these 'tandem' cells.

Through results published in *Nano Letters* in 2012, Dr Koleilat reported a greatly enhanced performance in tandem solar cell materials when impurities at precisely the right concentrations were introduced. Furthermore, her contribution to a study published in *ACS Applied Materials* in 2011 was instrumental in developing a device that converted over 3% of incoming sunlight into electricity – which was great performance for a solar cell based on quantum dots at the time. Both of these studies were widely hailed as major breakthroughs for the use of quantum dots in solar cell manufacturing, attracting praise from media groups including the National Post and MIT's Technology Review.



Record-breaking Performance

At the same time as this project, Dr Koleilat worked on new techniques for integrating her tandem solar cells into realistic power supply systems, paying particular attention to the composition of their constituent electrodes – the terminals that connect the solar cell to the electric circuit.

After a design had been perfected through computer modelling, the work resulted in a two-layer electrode – the first of which had a high concentration of impurities added, and supplied a high density of free electrons to an ultra-thin second layer of titanium dioxide. When integrated into a quantum dot solar cell by another student, Dr Koleilat's design achieved a record-breaking energy conversion efficiency of 8.5%.

In another study, published in *Scientific Reports* in 2013, Dr Koleilat explored the properties of quantum dots in a novel photovoltaic device design – a setup previously regarded as ineffective for realising efficient solar cells. Through her approach, however, Dr Koleilat enhanced the overall energy conversion efficiency by 30% compared with previous attempts.

Through each of these numerous and significant breakthroughs, Dr Koleilat has clearly demonstrated her prowess in developing innovative techniques for the integration of quantum dots into solar cells. Yet in her next few projects, she would demonstrate that her skills translate to an even broader range of technologies.

Sorting Carbon Nanotubes

After completing her PhD, Dr Koleilat began to explore further approaches to improving solar cell performance beyond quantum dots, through postdoctoral work at Stanford University. This time, her research focused on semiconducting carbon nanotubes – arrangements of carbon atoms wrapped into tubes just a few atoms thick.

In theory, these structures can improve energy conversion efficiency in similar ways to specialised dyes that are already widely used, and are known to significantly improve solar cell performance when placed between the layers of tandem cells.

Yet to achieve the same effect with carbon nanotubes, they must be precisely sorted – no easy task for such tiny structures.

Through research published in *ACS Nano* in 2014, Dr Koleilat and her colleagues devised yet another new technique for optimally sorting nanotubes in this way, which enabled extremely high yields of the structures. At the same time, her experiments brought about new discoveries regarding the transport of electrons across dual layers of nanotubes, providing researchers with new insights into how performance could be boosted even further.

Improving Perovskite Crystals

Following this work, Dr Koleilat investigated yet another approach to enhancing solar cell efficiency, involving thin films of a specialised composition – named 'perovskite'. When thin films of the material were deposited on top of existing solar cells in previous studies, researchers found that their electrical properties could be greatly enhanced. Dr Koleilat is now aiming to improve these properties even further, enabling perovskite films of only around 500 nanometres to 1 micrometre thick to be precisely deposited onto the surfaces of solar cells, to greatly enhance their performance at little cost to the manufacturer.

In her technique, reported in *ACS Photonics*, a thin film of perovskite is continuously blade-coated onto a moving surface. As it spreads, the perovskite film is smoothed out by a blade, to create a uniform film, creating macroscopic crystals with enhanced electrical properties. Like her previous breakthroughs, Dr Koleilat believes this blade-coating approach has the potential to transform the solar cell industry. However, several challenges remain before the technique can become widely commercialised.

Aims for the Future

Currently, the type of specialised perovskite used by Dr Koleilat quickly breaks down when exposed to air. Therefore, she now aims to find new ways to develop scalable, stable, and highly efficient devices incorporating the material, which are suitable for widespread integration into modern technologies. Having maintained a rapid pace of ground-breaking discoveries for over a decade, Dr Koleilat and the research team she now leads at Dalhousie University are in a stronger position than ever to realise these goals.

This work promises to strengthen the position of solar energy as one of the most advanced forms of electricity generation available. As renewable energy becomes an increasingly important aspect of the global energy generation mix, and the global fight against climate change gains momentum, Dr Koleilat's discoveries come at a critical time, and may soon prove to hasten our migration away from fossil fuels.



Meet the researcher

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Dr Ghada Koleilat completed her PhD in Electrical Engineering at the University of Toronto in 2012. Before graduating, she pioneered the use of quantum dots in solar cell manufacture, greatly improving their electrical properties. This technology is now patented and licenced to InVisage Technologies Inc. Upon completing her PhD, Dr Koleilat then embarked on her postdoctoral training at Stanford University, where she explored the potential use of carbon nanotubes in solar cells. Following this work, Dr Koleilat joined Dalhousie University as an Assistant Professor in 2016. She now leads the Koleilat Research Group at the university, which investigates the properties of advanced materials for use in advanced energy conversion technologies.

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Aurea Technologies

FUNDING

NSERC Discovery Grant

New Frontiers in Research Fund (Exploration-stream)

Canadian Foundation for Innovation

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ILLUMINATING PATHWAYS TO MORE RELIABLE PHOTOCONDUCTORS

Using laser light to produce and receive high-frequency radiation, photoconductors have become a promising aspect of materials science in recent years. So far, however, their production has faced a number of barriers. Through his research, **Dr Sascha Preu** at TU Darmstadt in Germany has tackled many of these challenges through the use of an alloy based on indium gallium arsenide enhanced with erbium arsenide particulates, whose electrons display some intriguing properties. His team's work has now greatly improved the prospects for photoconductors in applications including spectroscopy, imaging and non-destructive testing.

Photoconductors

Today, semiconductors are key components of some of today's most cutting-edge technologies, as well some of the latest research into materials physics. Although their compositions are highly varied, they are united by their characteristic property of increasing in conductivity as their temperatures rise, due to the resulting behaviours of their constituent electrons.

Through over a century of intensive research into their properties, physicists have now engineered semiconductor materials with a diverse array of highly specialised properties – each suited for particular tasks. Among these relatively new classes of materials are 'photoconductors' – whose electron properties are influenced by the light they absorb, instead of varying temperatures.

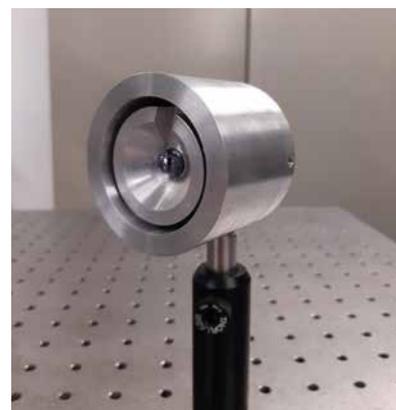
One particular advantage of these materials is their rapid change in conductivity when they are both exposed to and removed from sources

of laser light. As Dr Sascha Preu of TU Darmstadt explains, this property can be exploited to both produce and receive high frequency radiation. 'Photoconductors are semiconductor devices that feature a high resistance, that is switched to a low resistance by a laser signal,' he says. 'A high-quality photoconductive material recovers the state of high resistance within less than one picosecond, which is one trillionth of a second.'

In their research, Dr Preu and his colleagues aim to improve the performance of today's photoconductors beyond their current capabilities. As well as allowing for new techniques in spectroscopy, which they have already demonstrated in recent experiments, the team's work could offer new improvements for applications including spectroscopy, imaging, and communications systems.

Photoconductors in High-Frequency Systems

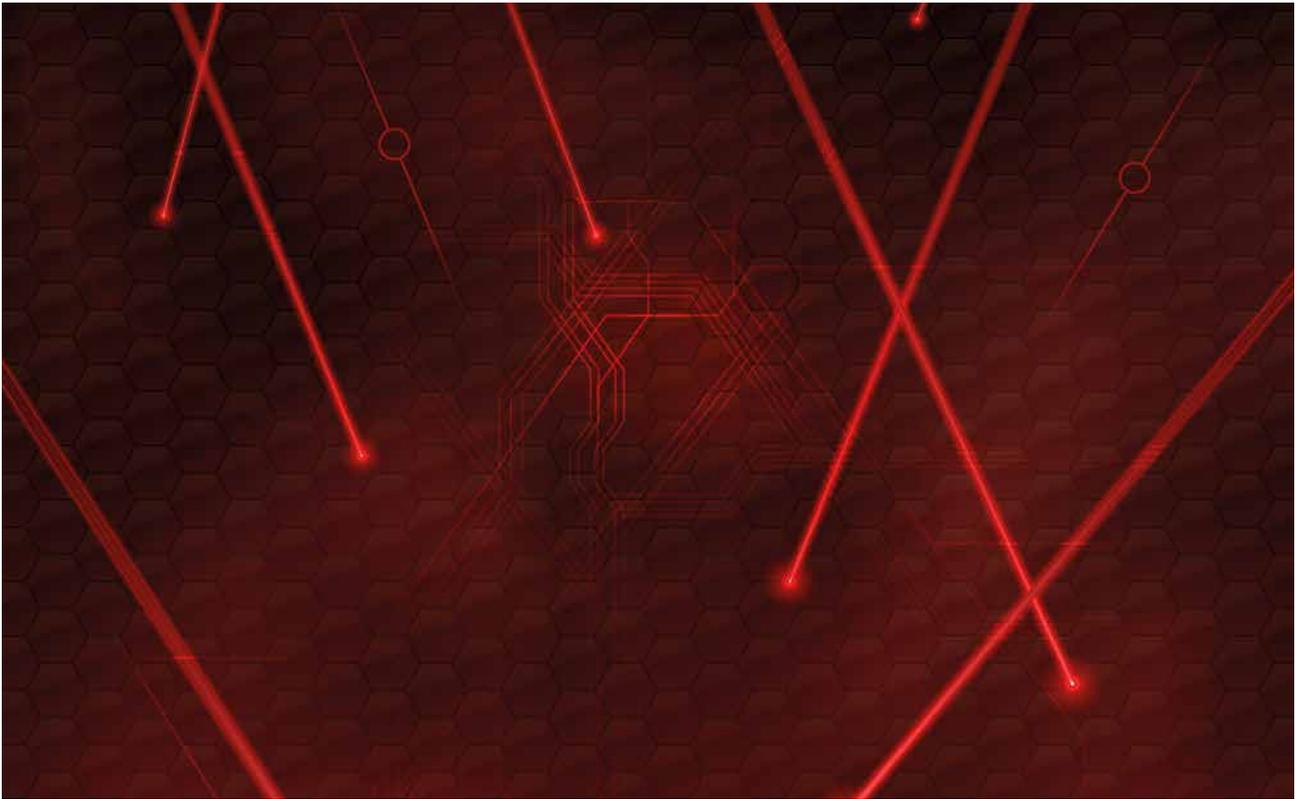
Before photoconductors can be made to produce and receive high



Photograph of a packaged photoconductive device

frequency radiation, some clever techniques are first required. In laser optics, a 'beat signal' describes the interference patterns that emerge between two beams with slightly different frequencies, giving a periodic variation in their collective brightness. Conveniently, the frequency of this variation is the very same as the frequency difference between the beams.

When such a beam pair strikes a photoconductor, the material's



electrons convert the beat signal into an alternating current, which changes direction at the same frequency as the frequency difference between the beams. Finally, an antenna attached to the material converts this current into ‘Terahertz’ radiation – which falls between the microwave and far infrared regions of the electromagnetic spectrum.

When driven by beat signals, these characteristics make photoconductors highly resistant to unwanted yet inevitable background noise. The inevitable background noise finally limits the minimum power that can be reliably recorded – known as ‘noise equivalent power’. Beat signals also allow photoconductors to reach high signal powers without the apparatus becoming overloaded. The ratio of the power in the system divided by the noise floor is referred to as ‘dynamic range’. Finally, they enable the materials to work within high frequency ranges.

Each of these values depends on whether the lasers are pulsed, or emitted in continuous beams.

‘Photoconductive devices play a vital role in light-dependent Terahertz systems,’ describes Dr Preu. ‘In continuous-wave systems, they serve as excellent receivers. In pulsed systems, they serve as both sources and receivers, offering frequency coverage of up to 7 Terahertz, and extremely high peak dynamic ranges beyond 100 decibels.’ Such receivers or ‘detectors’ of Terahertz radiation are invaluable in numerous technologies, including spectroscopy, astronomy and potentially communications.

Absorbing the Right Wavelength

Despite their numerous advantages, the development of reliable photoconductors is by no means an easy task for physicists. Critically, one particular wavelength of light is particularly well suited to fulfilling the potential of the materials: 1550 nanometre (nm) infrared radiation, which is a staple of many optical communications systems. While the light itself is easily attainable through commercially available laser-emitting diodes, making full use of it would prove more difficult.

To do this, Dr Preu’s team would need to construct a material which could reliably absorb the light, all while displaying just the right behaviours in its constituent ‘charge carriers’. These structures are formed when electrons are excited to higher energy levels, leaving behind a missing electron named a ‘hole’.

In a reliable photoconductor, electrons and their respective holes will move quickly when pulled along by an electric field, ensuring the highest possible conductivity when the material is illuminated. Yet at the same time, electrons must quickly fall back into their holes or engineered charge traps, and the material must become highly resistive when it is not being illuminated, ensuring the lowest possible conductivity in the dark. This way, the material can follow the modulation of the laser beat signal. ‘Further, it is challenging to engineer a material that offers high absorption at 1550 nm, sub-picosecond charge carrier lifetime, high carrier mobility, and high dark resistance – all at the same time,’ says Dr Preu.



Exploring a New Material

Since each of these properties is strongly influenced by material composition, the first major challenge for Dr Preu and his colleagues was to find a particular material which would be best suited to the task at hand.

Through studies carried out between 2010 and 2018, the researchers first experimented with a complex structure composed of erbium arsenide particulates within an indium gallium arsenide single crystal. To fabricate the material, they used a technique named 'molecular beam epitaxy', which is typically used in semiconductor manufacturing to deposit thin films of crystals. The films were grown by the researchers Hong Lu, Justin Norman and Arthur C Gossard at the University of Santa Barbara, California.

The resulting photoconductor, with the complex chemical formula ErAs:In(Al)GaAs , possessed many of the characteristics that Dr Preu's team were aiming for. By demonstrating short charge carrier lifetimes, high carrier mobilities, high absorption of electromagnetic radiation at 1550 nm, and high resistance in the dark, the team could finally satisfy their initial goals.

The next step in their research would be to prove the material's worth in real applications, particularly with respect to currently existing photoconductor technologies.

Satisfying Requirements

Having successfully fabricated their photoconductor, the researchers then rigorously tested its capabilities using theoretical models of the material. They also validated these results by comparing them to real experiments.

Through two further studies, carried out in 2017 and 2018, Dr Preu and colleagues showed for the first time that the requirements for light absorption, dark resistance, and charge carrier properties are all satisfied in ErAs:In(Al)GaAs . 'We have demonstrated that erbium arsenide-based 1550 nm photoconductors can fulfil the aforementioned challenges in an outstanding way,' says Dr Preu. 'We have achieved charge carrier lifetimes around and below half a picosecond, and extremely high dark resistance. This enables frequencies beyond 6 Terahertz in pulsed operation and continuous-wave frequency ranges beyond 3 Terahertz.'

The successful demonstration of these traits through both models and experiments then paved the way for feasible considerations of how the team's erbium arsenide-based material could be applied in real-world experiments and applications.

Applications in Spectroscopy

In a further 2019 study, Dr Preu's team demonstrated one particularly important application for their newly fabricated photoconductor. A technique known as 'time domain spectroscopy' typically involves probing the behaviours of materials when they are subjected to pulses of Terahertz radiation. Just like other spectroscopic techniques, the characteristic responses of the materials can reveal many of their physical properties, including their composition, conductivity, and optical behaviours.

Currently, time domain spectroscopy has shown a clear potential for applications including quality control in industries.

The study revealed that through the team's erbium arsenide photoconductor, pulses as short as 544 femtoseconds could be easily reached in practical telecom-wavelength operated time domain spectrometers that are both compact and inexpensive. The setup also allowed for single-shot frequency ranges as high as 4 Terahertz, and high peak dynamic ranges. All of this was made possible by the ability of ErAs:In(Al)GaAs to absorb the 1550 nm-wavelength light created by widely available laser-emitting diodes and erbium fibre lasers.

A Bright Future for Photoconductors

Through their watertight demonstrations of ErAs:In(Al)GaAs as a useful and reliable photoconductor, the findings of Dr Preu and his team have now opened up exciting new opportunities for these novel materials.

Beyond spectroscopy, their applications could include highly controllable resistors in electric circuits, accurate detectors of light intensity, and switches that operate using light instead of electric current. If applied to other situations where Terahertz radiation is commonly applied, they could be used to obtain non-invasive images of living tissues, search for concealed weapons, and transmit data.

Currently, the team applies the photoconductors within photonic vector network analysers and photonic spectrum analysers – a promising alternative to widely used electronic systems. A particular advantage of photonic systems will be the extraordinary frequency coverage in a single setup.

Through their continuing research, the researchers now hope to further improve the capabilities of low-cost photoconductor-based systems, allowing their techniques to become even more competitive in the future.



Meet the researcher

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Dr Sascha Preu completed his doctoral degree at the Max-Planck Institute for the Science of Light and FAU Erlangen-Nuremberg in 2009. He continued his work at the University of California, Santa Barbara, as part of a Humboldt Feodor Lynen fellowship. After working as a postdoctoral associate at FAU Erlangen-Nuremberg, he became assistant professor at the Department of Electrical Engineering and Information Technology of TU Darmstadt in 2014, leading the Terahertz Devices and Systems Group. In 2018, he was promoted to a full professor. In his work, Dr Preu focuses on the development of Terahertz sources and detectors, including photoconductive materials. He also focuses on terahertz detection through specialised transistors and system-level applications, including photonic vector network analysers and photonic spectrum analysers. His research has now earned him numerous awards including the European Research Council's ERC Starting Grant, which he received in 2017.

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FUNDING

Deutsche Forschungsgemeinschaft (DFG), Project No. 278381540 (REPHCON)

European Research Council (ERC), Grant Agreement No. 713780 (Pho-T-Lyze)

Horizon 2020 innovative training network 'CELTA' Grant agreement number 675683

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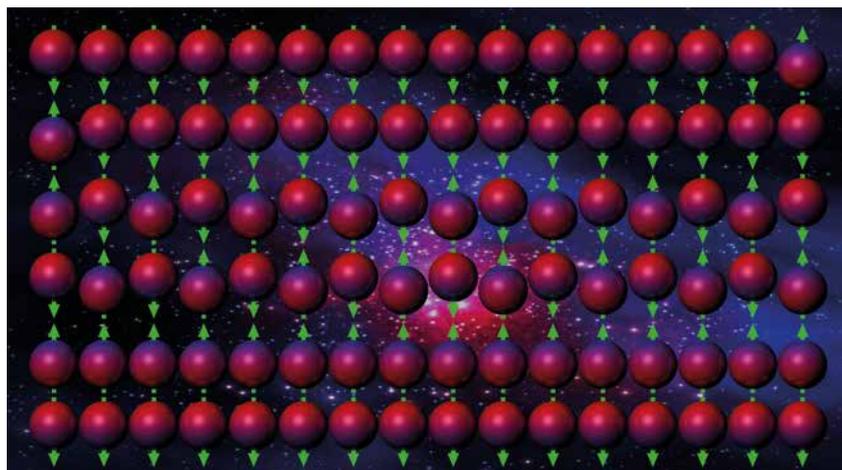
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CONTROLLING LIGHT BY MANIPULATING ELECTROMAGNONS

Within some specialised materials, light can appear to move in mysterious ways, rotating around its direction of propagation, and becoming dimmed to different degrees, depending on its direction of travel. **Professor Andrei Pimenov** and his team at the Vienna University of Technology investigate how these properties are linked to recently discovered quasiparticles named 'electromagnons'. The team's work could soon open up new ways to consciously control the propagation of light within these unique solid materials, with numerous exciting technological applications.



using light. These collective spin excitations, known as magnons, have some interesting and potentially useful properties.

Magnons are commonly found in a class of materials named ferromagnets, in which the alignment of their constituent atoms' magnetic properties means that they remain magnetised permanently. They also appear in other classes of materials, displaying properties called ferroelectricity and ferroelasticity; together, these three classes are named 'ferroic' properties. Within these materials – originally composed of iron as their name suggests – magnons can influence a variety of properties, including conductivity and heat transfer.

As techniques to study the properties of magnons improve, their potential applications are becoming increasingly apparent. In particular, they show promise in forming a basis for highly compact transistors, which carry out operations on collective excited electron spins. In addition, researchers are finding new ways to store information on these collective spins; opening up new routes towards highly compact hard drives.

Quasiparticles

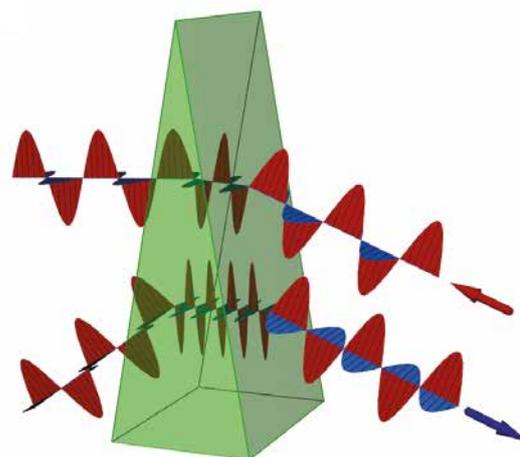
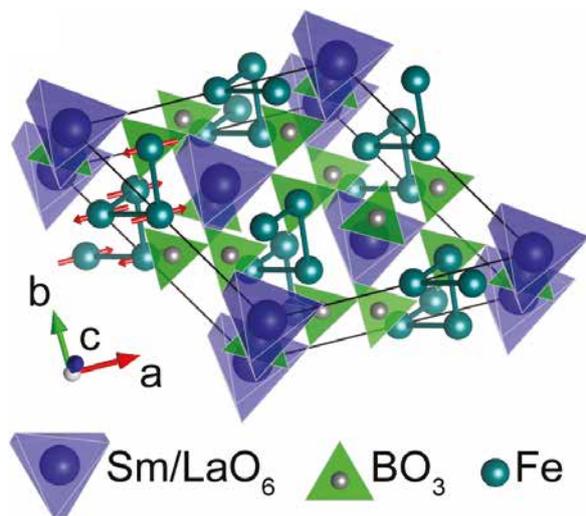
Within a variety of solid materials, certain particles, such as electrons, can adopt disguises as they move around. Known as 'quasiparticles', these structures might appear to an observer to act like new particles with completely unique properties. However, since the behaviours of quasiparticles are simply a result of the influence of the surrounding 'real' particles they interact with, they remain completely within the bounds of the laws of physics.

Important for a variety of technological applications, quasiparticles represent

a diverse family of structures, including phonons, plasmons, and fascinating phenomena called magnons.

Properties and Applications of Magnons

Among several other quantum properties, an individual electron possesses a value named its 'spin', which is analogous to the angular momentum of a rotating object on a quantum scale. Electron spins usually behave independently of one another, but in the right conditions, the spins of groups of electrons can be been collectively excited to the same energies



However, through the use of increasingly specialised ferroic materials, Professor Andrei Pimenov and his team have discovered that magnons can display even more intriguing properties, pushing these potential applications to new limits.

Uncovering Evidence for Electromagnons

In 2006, Andrei Pimenov, then working at the University of Augsburg in Germany, carried out a novel series of experiments with ‘multiferroic’ materials, which display at least two of ferroic properties. Most commonly, these materials are both ferromagnetic and ferroelectric, meaning that both their magnetisation and the alignment of their constituent atoms, or ‘polarisation’, can be switched by applying magnetic and electric fields, respectively. These substances are particularly interesting since their magnetic properties, and their degree of polarisation in applied electric fields – or their ‘dielectric’ properties – are strongly linked, earning them the name ‘magnetodielectric’ materials.

In their study, Andrei Pimenov and his colleagues applied alternating electric fields across two different multiferroic materials: terbium manganite and gadolinium manganite. They found that the magnons present in these compounds could be excited and observed only if the spins of manganese ions were arranged in form of a spiral.

However, when an external magnetic field was applied, which forced all manganese spins to become aligned parallel to the field, thus destroying the magnetic spiral, these magnons disappeared.

Since these unusual quasiparticles were excited by electric fields of light contrary to regular magnons, the researchers dubbed them ‘electromagnons’. In the coming years, they would become an important basis for Professor Pimenov’s research.

Anisotropy and Polarisation Rotation

One particularly mysterious property also arose in the magnetodielectric materials themselves. It was observed that the light propagating through the materials appeared to be asymmetrical – an effect named ‘directional anisotropy’. This meant that instead of propagating evenly, as would be the case within a regular block of uniform glass, two light beams travelling in opposite directions within a multiferroic material would be absorbed differently – being slowed down to different speeds. Indeed, the team showed that light can be completely stopped along one direction, and allowed to travel freely in the other, by fine-tuning the geometry of an external magnetic field.

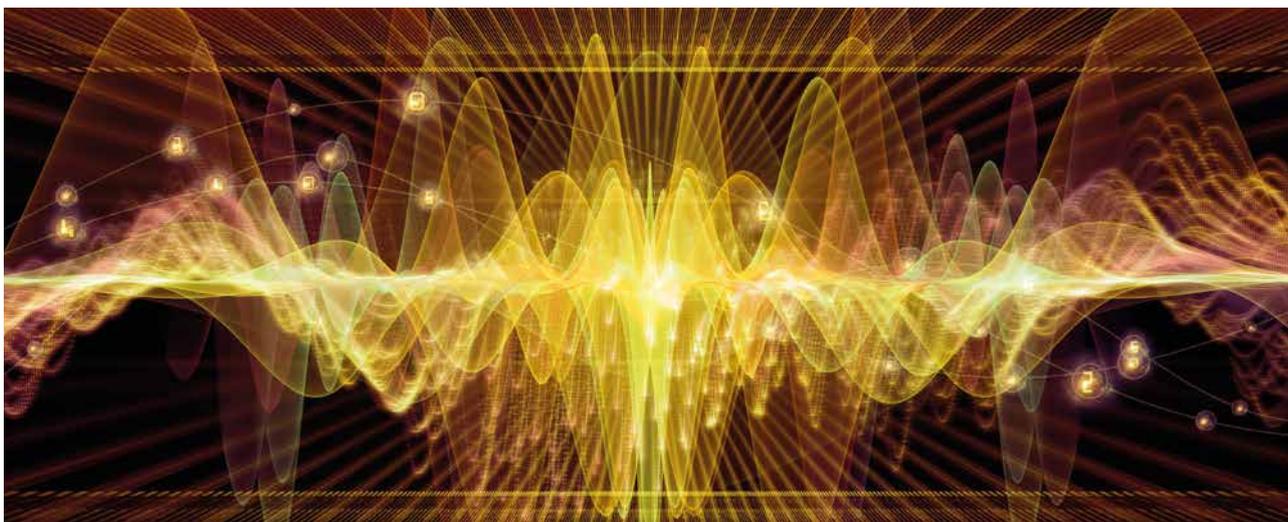
In several other studies, Andrei Pimenov’s team also explored changes in linearly polarised light, whose constituent fields vibrate in one

specific direction, as it travels through multiferroic substances. They found that regardless of the frequency of the light, the direction of this polarisation will rotate around the light’s direction of travel. Furthermore, just as the anisotropy of a magnetodielectric material can be tuned using an external magnetic field, the researchers discovered that both the amplitude and direction of this polarisation direction can be tuned using an external electric field.

Manipulating Excitation

Having demonstrated these capabilities for optical property manipulation using external fields, Andrei Pimenov and his colleagues next aimed to show how they could be used to influence the behaviours of electromagnons.

In their initial experiments, the team did not know enough about the properties of electromagnons to explore how they could be formed under different conditions. However, in further studies, they realised that external electric and magnetic fields can alter the frequencies at which the quasiparticles become excited. Shifting the frequencies of magnetic processes in this way is a key barrier to overcome for many experiments in materials physics, especially those with applications in electronics.



In this case, the physicists were able to identify a series of magnetic vibrations within the constituent molecules of a particular class of multiferroics named iron borates, which were sensitive to both electric and magnetic fields at the same time. This sensitivity arose because the directions of the magnons' collective electron spins were modified by the fields. In turn, this altered the characteristic frequencies at which the magnons were excited.

Having uncovered this mechanism, Professor Pimenov's team could finally excite electromagnons within magnetodielectric materials, at the terahertz frequencies they required for their experiments.

Controlling Light with Electromagnons

At the same time as these studies, Professor Pimenov and his colleagues explored the reverse situation: how electromagnons themselves could be used to influence the properties of external fields. Their previous studies had already revealed an intrinsic coupling between the quasiparticles and external electric and magnetic fields, which themselves were shown to influence polarisation rotation and anisotropy, respectively. Therefore, the next logical step in this line of research was to use electromagnons to precisely control the properties of light passing through magnetodielectric materials. In the final step of this puzzle, the physicists investigated how the characteristics of electromagnons in magnetodielectric materials were linked to these properties.

Andrei Pimenov's team discovered that variations in both anisotropy and polarisation rotation showed substantial responses close to the resonant frequencies of electromagnons – the frequencies at which the electron spins collectively display the strongest responses to external electric and magnetic fields. Specifically, the researchers observed that the 'transmission coefficient' of magnetodielectric materials – the total power of waves that have passed through, in proportion to the waves that first entered – began to differ hugely in forward and backward directions, in the vicinity of these frequencies.

In addition, linearly polarised light entering the materials rotated by an angle proportional to a value called the 'magnetolectric susceptibility', which describes how the material becomes electrically polarised in response to a magnetic field, and vice versa. Again, the team observed that the angles become larger close to electromagnon resonance frequencies.

By fine-tuning the properties of their electromagnons using external fields, and through careful selection of multiferroic composition, the researchers were able to demonstrate high degrees of control over the light traveling through magnetodielectric materials. This highlights that since their discovery in 2006, electromagnons have gone from being a mysterious new type of quasiparticle, to a well-understood and useful tool for controlling the propagation of light.

A Bright Future

The work of Professor Pimenov and his colleagues has now broken down many of the mysteries surrounding the unusual properties of magnetodielectric materials, and the electromagnons they contain. The ability to control the polarisation rotation and propagation asymmetry of light travelling through the materials could have incredibly useful optical applications, providing new opportunities for experiments and technologies alike.

In particular, more sophisticated techniques for control using electromagnons could open up new and innovative routes towards highly compact transistors and data storage devices in quantum computers in the near future. For now, Andrei Pimenov's team will continue to explore the rich variety of intriguing properties observed in multiferroics and other magnetodielectric materials, and will aim to learn more about the unusual behaviour of electromagnons.



Meet the researcher

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Professor Andrei Pimenov studied physics at Moscow Institute of Physics and Technology, and received his PhD degree from the Technical University of Darmstadt in 1995 for a dissertation on dynamic conductivity of superconductors using contact-free methods. In 2001 he did his Habilitation in experimental physics with the title 'Submillimetre-Wave Electrodynamics of Superconductors' at the University of Augsburg. In 2006, he became Associate Professor at the University of Würzburg, where he worked until 2010. He is now a full Professor at the Vienna University of Technology, where he leads the Solid-State Spectroscopy group. Here, he is also the Director of the Institute for Solid State Physics. Professor Pimenov has authored more than 120 papers in several fields of solid-state physics, spectroscopy and metamaterials. He is married and has two children.

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ION-BARRIER COATINGS: THE NEXT GENERATION OF ANTICORROSION TECHNOLOGY

Corrosion, the gradual destruction of metals, is a significant physical and economic problem worldwide. Traditional heavy metal-based coatings used to protect metals are now viewed negatively due to their impact on the environment. Research led by Jianguo Wang of AnCatt Inc reveals why ion-barrier coatings are the next generation of anticorrosion coating technology.

Economic and Environmental Costs

Anybody who neglects oiling their steel bicycle chain, particularly after being subjected to rain, will soon notice the once shiny metal turn into a deep orange brown. This is an example of corrosion – the natural, gradual destruction of metals. Iron within the bicycle chain reacts with oxygen and moisture to form iron oxides, or rust, and the once useful properties of the steel, including strength and appearance, are modified. Left alone, this surface corrosion causes pits and cracks, finally rendering the metal useless.

According to a report issued by NACE International, metal corrosion causes \$2.5 trillion USD in losses globally each year, in the order of 2–3% of gross national product (GDP). Therefore, protective coatings for metal are extremely important.

Historically, coatings containing lead and chromates have proven to be successful, but are now considered environmentally poisonous. Chromate-containing anticorrosion coatings, once

used extensively within the aircraft, automotive, construction and marine industries, are now known to be human carcinogens. The EU banned their use in the automotive industry in 2007 and these coatings are under increasing scrutiny worldwide, which creates a need for non-toxic and environmentally benign alternatives. Zinc is another common metal used in anticorrosion coatings; while it is less toxic, this heavy metal is also less effective and cannot protect aluminium from corrosion.

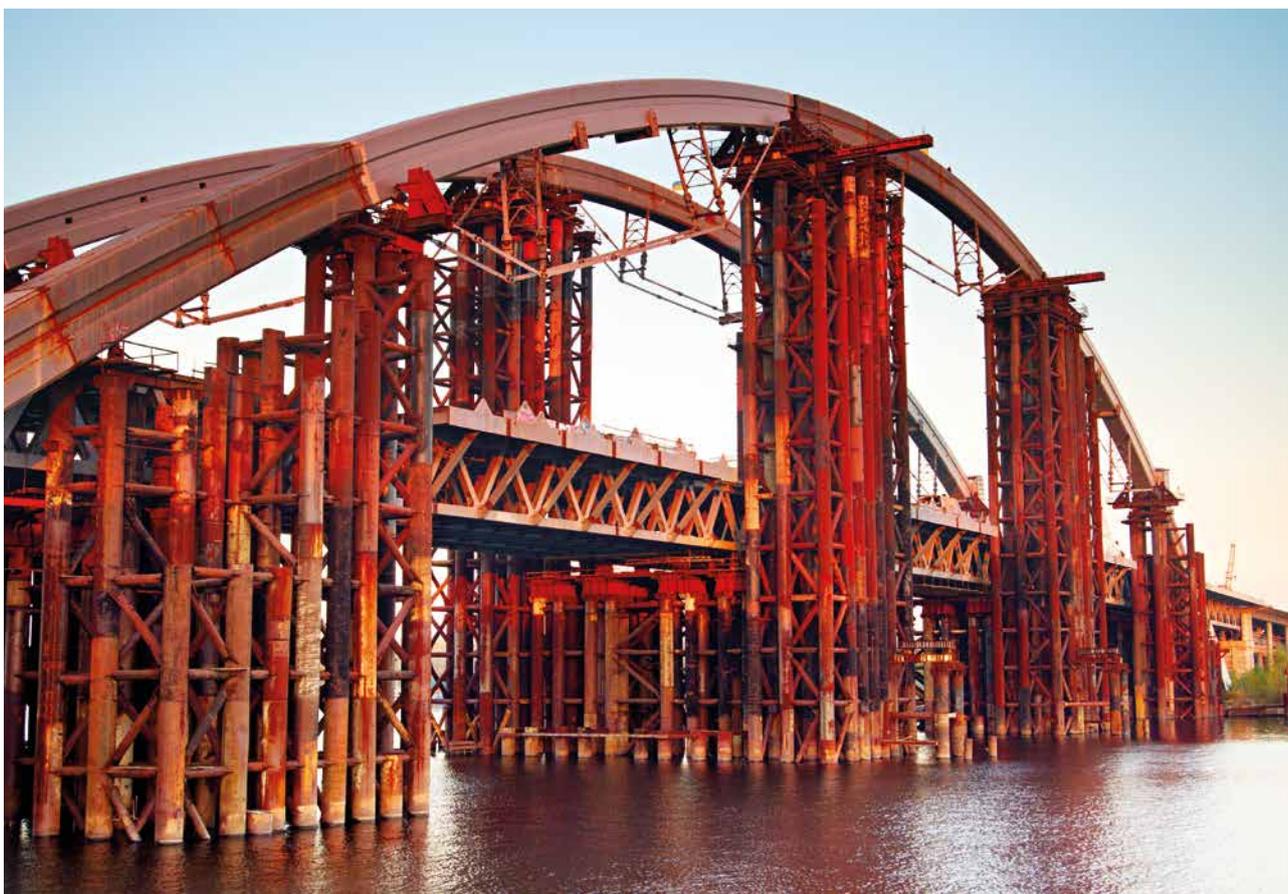
Insights into Polyaniline

Newly-developed coatings based on an organic polymer called ‘polyaniline’ are exciting due to their effectiveness at preventing corrosion and their relatively benign impact on the environment. Although discovered over 150 years ago, attention from the scientific community remained low until the 1980s, when the material’s high electrical conductivity was rediscovered and its anticorrosive effect was observed.

Based on its anticorrosive properties, a German company called Ormecon GmbH developed a polyaniline paint



product called Corrpasiv™. Soon after, many scientists attempted to understand the corrosion protection offered by doped polyaniline based on its conductive nature. Many research papers were published and several patents were issued. Then, in 2008, Enthone Inc announced the acquisition of Ormecon GmbH, and their aims to pursue other applications of polyaniline. Unfortunately, Enthone Inc decided



not to continue the development of polyaniline anticorrosion coatings, indicating that there were challenges associated with their development.

Jianguo Wang, a chemist, began studying polyaniline coatings in 1993 at Drexel University in Philadelphia. Wang joined the DuPont Chemicals Company in 1995 (now DowDuPont Inc) and, although focused mainly on other projects, continued to study polyaniline as a side project. His aims included understanding the chemical structure of polyaniline and its anticorrosion mechanisms. He left DuPont in 2008 and founded the Ancatt Company, which has now successfully formulated anticorrosion coatings based on conducting organic polymers.

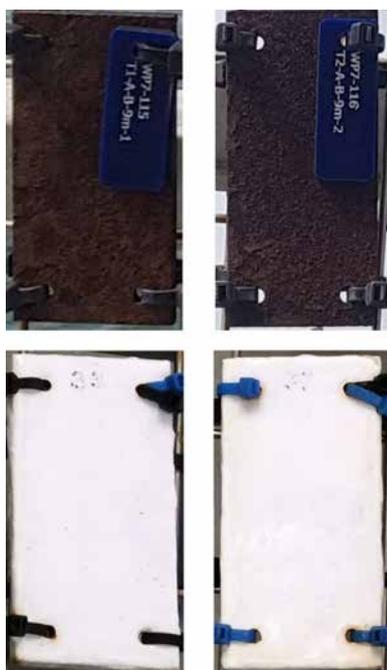
There are two basic forms of polyaniline materials – a conducting form and an insulating form, known respectively as emeraldine salt and emeraldine base. The corrosion prevention effect of the conducting form has been known since the 1980s, attributed to its metallic-like properties. However, it was more surprising to find that anticorrosive properties are also present in the insulating base form, even outperforming the salt in certain circumstances. Furthermore, chemical analysis of the emeraldine base conflicted with the structure that was accepted at the time for this compound.

Wang investigated these discrepancies and published his results in a paper in early 2002. By adding emeraldine base powder to various salt solutions, he observed that the presence of emeraldine base modifies the nature of the salt present. Emeraldine base, he realised, acts as an ‘anion’ exchanger. Anion is the name given to a negatively charged ion, whereas cations are positively charged. In simple terms, emeraldine base exchanges anions within its structure with anions in the salt. Wang concluded that emeraldine base must have a different structure to the one that was accepted, and proposed a new chemical formula and structure. He also concluded that it is the material’s anion exchange behaviour that partially explains the anticorrosion properties of the material.

Further Experiments

Later that year, Wang published research investigating further the anticorrosive properties of polyaniline. In his experiment, he applied different configurations of polyaniline coatings, of the same thickness, to steel panels and measured the corrosion protection offered in terms of the ‘pore resistance’ – a measure of how ions flow through the material.

One of the coatings applied, termed ‘bipolar’, consisted of a polyaniline layer applied directly to the steel surface and a cation-exchanging layer applied on top (a topcoat). A second ‘non-polar’ coating consisted of a single layer of the two materials mixed together, and a third consisted solely of a single layer of polyaniline.



Top: Bare panels exposed to the atmosphere for 7 months. Bottom: AnCatt coated panels exposed to the atmosphere for 1 year.

The 'bipolar' layer offered the best protection in terms of preventing corrosion, attributed to the polyaniline forming a barrier to positively charged metal cations, whilst the topcoat forms a barrier to aggressive negatively charged anions interacting with the metal. Effectively, the bipolar coating acts as an 'electronic barrier' to both cations and anions, and hence the 'pore resistance' has a high value.

On the other hand, single-layer polyaniline coatings are permeable to aggressive anions and hence have limited lifetime in preventing corrosion. With the two layers mixed in the non-polar layer, the coating is permeable to both anions and cations, and the anticorrosive ability is negligible. In a comparison of the base and salt form of polyaniline, Wang concluded that emeraldine base is a stronger anticorrosive material than emeraldine salt when a topcoat is absent.

Wang, together with Charlie Torardi and Michael Duch, fellow colleagues at DuPont, published research in 2006 that further examined the anticorrosive

properties of polyaniline by applying various coatings to filter paper to make membranes. To assess the anticorrosive properties, they measured how easily charged particles move across the membranes. Wang's conclusions from these experiments agreed with his earlier 2002 study. Bipolar layers form barriers to cations and anions and hence they have an increased ability to prevent corrosion. Mixed layers result in imperfections, reducing their ability to protect against corrosion.

A second aspect of the team's research involved coating steel panels, as Wang had done in his 2002 study, but this time adding a 'reverse bipolar' coating – a cation-exchanging layer coated on the metal first with polyaniline used as a topcoat. As found in the 2002 study, single-layer polyaniline coatings impede the movement of cations but cannot prevent the passage of aggressive anions such as chlorides (found in salt). Again, they found that the bipolar layer is most effective due to its dual behaviour of preventing anions and cations permeating through.

Delamination of organic coatings, where the material breaks by fracturing into layers and separates from the metal surface, is one of the most common forms of failure and occurs when cations enter the coating-metal interface. Hence, single-layer coatings consisting solely of a cation exchange resin that is permeable to cations are ineffective, as are 'reverse bipolar' coatings when the cation exchange resin is applied to the metal surface first.

Next Generation Coatings

Since founding the AnCatt Company based in Newark, Delaware, Wang and his colleagues have successfully developed award-winning, heavy metal free, highly effective anticorrosion coatings for metals. AnCatt claims that their coatings are ion-barrier coatings, which combine a primer that acts as a barrier to cations with a topcoat that acts as a barrier to anions. The primers include, but are not limited to,

polyaniline coatings. These ion-barrier coatings are expected to be the next generation of anti-corrosion coating technology.

In a 2017 study, Wang and his colleague Sue Wang compared AnCatt's ion-barrier anticorrosion coating to commercially available zinc-rich and zinc phosphate coatings. They applied different coatings to steel panels, scratched them down the middle and exposed them to a 'salt-fog' – a quality control widely used within the paint industry.

An independent company employing standardised corrosion rating systems evaluated the damage after 700 hours and 2000 hours of exposure. After 700 hours, the level of corrosion with AnCatt's ion-barrier coating applied was almost equal to that observed with commercially available zinc-rich paint, but corrosion was notably less after 2000 hours. In fact, there was essentially no difference in corrosion between 700 hours and 2000 hours when employing the ion-barrier coating.

Using the standardised measuring systems, all the coatings received a perfect 10 for 'Red rust rating' and 'Blister rating' but the ion-barrier coating performed 1–3 points higher (on a scale of 1 to 10) for 'Scribe rating' than the commercially available coatings.

A Lustrous Future

Through over 25 years of leading research starting with the organic polymer polyaniline, Jianguo Wang has provided insights into ion barrier coatings, and the reasons behind their effectiveness as an anticorrosive coating for metals. As we move away from the use of traditional heavy metal-based coatings due to their deleterious impact on the environment and human health, ion-barrier coatings have a bright, lustrous future.

Meet the researchers



Mr Jianguo Wang
AnCatt Company
Newark, Delaware
USA

Mr Jianguo Wang was awarded his MS degree from Peking University in China in 1982. In 1993, he began research into the anticorrosive properties of conducting polymer materials, within the group of Professor Yen Wei at the Drexel University in Philadelphia. Wang joined the DuPont Chemicals Company in 1995, where he focused on other projects, but continued to study the anticorrosive properties of organic polymer materials, with a particular focus on polyaniline. On leaving DuPont in 2008, he founded the AnCatt company in Newark, Delaware. AnCatt successfully developed ion-barrier anticorrosion coatings, receiving grants from the National Science Foundation and several other prestigious awards.

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Ms Sue Wang

Ms Sue Wang received her bachelor's degree in Computer Science from the University of Delaware and MBA from Godey Beacon College. Ms Wang is currently the CEO of the AnCatt company. She led AnCatt to win the American Chemical Society Green Chemistry Challenge, the TechConnect National Innovation Award, the Most Promising Energy and Clean Tech Company venture award by the RICE ALLIANCE, and NASA's LAUNCH Green Chemistry Award.



Ms Nar Wang

Ms Nar Wang is the Chief Operating Officer (COO) at the AnCatt company for over 8 years. She received her bachelor's degree in China.

KEY COLLABORATORS

Charlie C. Torardi, inorganic chemist

Michael W. Duch, ESCA expert

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FUNDING

US National Science Foundation (2015–2018)

FURTHER READING

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ANAM2019: SHOWCASING NANOSCIENCE & FOSTERING INTERNATIONAL COLLABORATION

The field of nanomaterials has exploded in recent years, and perhaps the main pillar of its success has been a close collaboration between institutions and research groups across the globe. In September 2019, **Dr Habil Souren Grigorian** at the University of Siegen, Professor Ishkhan Vardanyan at Yerevan State University and their colleagues organised an event that showcased Armenia's growing interest in this area of research. Following a week of activities widely praised by its participants, the Advanced Nanomaterials and Methods (ANAM) 2019 International Workshop and Young Scientist School promises to spark further innovation in nanomaterials research in Armenia and the surrounding regions.



Facilitating Knowledge Exchange

Within a field as diverse and complex as nanoscience, new advances are far more likely to be made through exchanges of knowledge between researchers from widely varying backgrounds. With this in mind, Dr Souren Grigorian of the University of Siegen, Professor Ishkhan Vardanyan of Yerevan State University and their collaborators set out to extend this network within Armenia and facilitate opportunities for nanomaterials research, which is currently spearheaded by Yerevan State University (YSU).

On September 25th, 2019, YSU's Departments of Molecular Physics and Solid State Physics opened ANAM2019, hosting a diverse array of nanomaterials researchers across the globe.

'ANAM2019 aimed to bring together leading scientists and researchers from different fields of nanomaterials and nanocomposites, as well as their characterisation methods on various scales,' describes Dr Grigorian. 'Our aim was to create new scientific links in this novel and fast-developing field in Armenia and the neighbouring countries of the region. The multidisciplinary

of ANAM2019 brought together experts and scientists from nanotechnology and nanoscience, with backgrounds in complementary fields: chemistry, physics, biology, medicine and material science.' The announcement of ANAM2019 received strong interest from the scientific community, with over 100 participants from more than 12 countries – ranging from USA to Singapore.

To strengthen these links further, and to inspire future innovations, the event also served to connect world-renowned researchers with promising students in the field. 'Many students and young scientists had the possibility not only to attend lectures, but also to have direct contact with these invited world-renowned speakers,' Dr Grigorian continues. 'We have received a lot of positive feedback concerning the ANAM2019 events from experts, as well as from students.'

'The multidisciplinary of ANAM2019 brought together experts and scientists from nanotechnology and nanoscience, with backgrounds in complementary fields: chemistry, physics, biology, medicine and material science.'



This sentiment was shared by four particular participants with widely varying backgrounds – from a Masters' student just starting out in the field, to experimentalists with decades of experience. Next, we'll discuss the research of these four individuals and highlight their experiences of ANAM2019.

Understanding Biology with Nanotechnology

Dr Sergio Moya is a group leader at CIC biomaGUNE – a non-profit research organisation based in San Sebastian in Spain. His group is dedicated to using nanotechnology to understanding biological systems on microscopic scales.

At ANAM2019, Dr Moya presented a study on biomaGUNE's latest research into 'polyelectrolytes' – polymer nanoparticles hosting repetitive chains of charges. His study explored the numerous advantages of these structures, including their ease of synthesis and assembly, their strong responses to their surrounding environments, and their suitability for hybrid materials and coatings. Later, Dr Moya gave a talk detailing the urgent need for a deeper understanding of the impacts of engineered nanotechnologies on human health

– both through nanomedicines, and through accidental exposure.

Dr Moya praises the social aspects of ANAM2019, which allowed him to interact with researchers he has known and worked with throughout his long career, while at the same time, gaining new perspectives.

'For me, ANAM2019 was an interesting opportunity to meet old and new friends, while discussing science at a high level,' he recalls. 'I had great fun during the meeting and enjoyed the varied topics presented. From the perspective of the Armenian students, both graduate and undergraduate, it was very useful to be exposed to different scientific topics and scientists from all over the world in a very relaxed and friendly environment.'

Nanomaterials for Advanced Technologies

As an Associate Professor at the Sapienza University of Rome, Professor Ilaria Fratoddi aims to develop new nanomaterials for advanced technological applications, including sensors, nanomedicines and biotechnologies. Her methods for producing these materials including chemical synthesis, and structural and functional studies of existing nanomaterials.

At ANAM2019, Professor Fratoddi presented a study on how the properties of nanoparticles can be fine-tuned by controlling their size, shape, composition, order, and structure. She also gave a talk on the versatile and controllable optical properties of nanoparticles synthesised using corrosion-resistant metals, for applications including catalysis and energy conversion.

Like Dr Moya, Professor Fratoddi also relished the social aspects of the event, and was particularly impressed by the scope of scientific topics that were covered within the wider field of nanomaterials.

'ANAM2019 was a really interesting and well-organised opportunity to share scientific results in a friendly context,' she describes. 'The organisation was excellent, and the choice of speakers covered different scientific fields. This gave a real multidisciplinary approach to material science, and at the same time, was an informal and open-minded opportunity.'

Even with her years of experience in the field, Professor Fratoddi felt that the interactions facilitated by the events presented her with fresh new ideas for her research. 'The school and meeting gave me the chance to look at



high-level research by scientists from different backgrounds,' she continues. 'I enjoyed listening to the very recent scientific results of colleagues, and on occasion, to find new connections and to improve or start new collaborations.'

Supporting Students

Perhaps the one aspect of ANAM2019 most celebrated by its participants was the open inclusion of students, just starting out in their careers in nanomaterials. 'One of the things I appreciated was the contributions from young students, who presented their first results and had the chance to compare their results with those of other scientists,' Professor Fratoddi adds. 'The warm hospitality and the attention to every detail made this meeting one of the best in my experience.'

One such participant was Varazdat Stepanyan, a Masters' student at YSU, who alongside Dr Moya, Professor Fratoddi and their distinguished colleagues, presented a study regarding interactions between polyelectrolytes. In the talk, he highlighted how calculations of these interactions can be made more accurate through particular mathematical approaches.

Stepanyan and his peers particularly benefitted from the Young Scientist School aspect of the event, which ran alongside the main workshop. Through both academic and social events, the school enabled prospective nanomaterials researchers to forge relationships, which would prove invaluable in helping them to break into the field.

'As a student participating in ANAM2019 I can say that it was a wonderful experience,' Stepanyan expresses. 'The school was very useful as we had the opportunity to both attend lectures and give short speeches about our research. Not only was the scientific part of the school and workshop organised very well, but the entertainment activities were also excellent, which helped the younger participants form a connection with the elder participants.'

Diverse Topics, Common Methodology

Also attending YSU as a PhD student, Arevik Asatryan joined Professor Fratoddi in praising the diverse variety of research areas presented at ANAM2019. 'Participation in both school and workshop was an incredible experience for me,' she says. 'I got the opportunity to learn from scientists from all over the world, who work in various fields: from solid state physics to biophysics and physical chemistry. The topics varied from physical methods of investigations to pure biological research. Despite the diversity of the topics, the methodology used was common.'

As part of the workshop, Asatryan and her colleagues presented three of their recent studies – two of them detailing how biological polymers transition from states of order, to states of disorder. This involved calculating the free energy of polymer nanoparticles, derived from multiple different monomers, using new techniques. In turn, other parameters of these nanoparticles could be calculated afterwards. In addition, Asatryan reported new insights into the properties of quantum wires, which are so thin that the ways in which they conduct electricity are influenced by quantum effects.

Asatryan describes how ANAM2019 allowed her to promote her achievements among established researchers, while finding answers to pressing issues which had been holding back her research. 'I was able to find answers to questions not only from my field but also from other fields,' she continues. 'Moreover, I found out about another experimental method for structural investigations of macromolecules, which may help us in the future in order to compare the results. I also made some connections with the professors whose research topics and specific investigations were very interesting for me. This may even lead to future collaboration.'

Inspiring Future Innovation

ANAM2019 concluded on October 2nd following a week of presentations and workshops, but its impact will almost certainly be felt within the wider field of nanomaterials well into the future. As Dr Habil Grigorian concludes, the widespread consensus among participants was that the event was a resounding success.

'We expect that with a strong contribution of international experts and leading scientists, ANAM2019 will have served as a platform for networking,' he says. 'It has also initiated joint research projects, which could help to facilitate the development of young scientists, and to influence their future research.'

ANAM2019 now places Armenia among the diverse nations making significant contributions to nanomaterials research, strengthening the prospects for this exciting field even further.



Meet the researchers

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Dr Habil Souren Grigorian completed his PhD in Physics at the Institute of Crystallography, Russian Academy of Sciences in Moscow in 2000. He has since held a variety of research positions at institutions across Europe and became head of the Soft Matter Physics Group at the University of Siegen in 2010. For his work in developing a novel concept for in-situ studies, he was awarded his French Habilitation in the chemistry of materials at the Université de Haute-Alsace, Mulhouse-Colmar-Strasbourg in 2015. As an internationally recognised researcher, he was offered the role of invited professorship at Aix-Marseille University, France, in 2016 and has also been a visiting professor at Sapienza University of Rome, Italy, in 2018. Among his research interests are advanced x-ray techniques for investigating multifunctional soft materials, in-situ studies of working organic devices, direct correlation of microstructures and optoelectronic properties, and flexible organic electronics. Outside of his research, Dr Habil Grigorian has actively participated in teaching on an international level, and has coordinated the Volkswagen Foundation's grants for the International Symposium and Young Scientist School over several years.

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Professor Vardanyan completed his PhD in Molecular Physics at Yerevan State University in 2012. He has since worked in the university's Department of Molecular Physics as assistant professor, and has worked as an invited researcher many times at institutions including Leipzig University in Germany, and CIC BiomaGUNE in Spain. His main research interests include the thermostability and conformation of biopolymers under different conditions and the interaction of biopolymers with different ligands, as well as nanoparticle diffusion. Alongside his research, Professor Vardanyan has been heavily involved in a variety of young scientist support programmes, and also became the Head of Yerevan State's Scientific Policy Department in 2017.

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FUNDING

Volkswagen Foundation
Ministry of Education, Science, Culture and Sport of RA
Yerevan State University



PHYSICS

QUANTUM LEAPS IN PHYSICS RESEARCH

In the final section of this exciting edition, we home in on the nuts and bolts of our physical reality. Here, we highlight a diverse mix of fascinating research projects, each dedicated to unravelling how matter behaves at its most fundamental level, while also laying the foundation for revolutionary technologies.

To open this section, we feature an exclusive interview with Dr Matthew McCullough, physicist at the famous particle physics research centre, CERN. Here, Dr McCullough discusses CERN's plans to build a new particle accelerator that is almost four times longer than the Large Hadron Collider – currently the world's most powerful accelerator. This new Future Circular Collider will be able to accelerate particles to unprecedented speeds, leading to collisions that will allow scientists to look even deeper into the microscopic innards of nature.

Professors Klaus Peters, Miriam Fritsch and Wolfgang Gradl in Germany have also dedicated their research careers to understanding the behaviour of subatomic particles. By investigating how quarks bind to each other within protons, neutrons and larger 'multi-quark' particles, the team is working towards solving some long-standing mysteries in particle physics.

In the third article of this section, we shift our focus to the atomic nucleus of Thorium-229, a variant of the element thorium. Here, we showcase the work

of Dr Peter Thirolf and his colleagues at Ludwig-Maximilians University Munich, who have been exploring the quantum structure of this atomic nucleus in great detail. After characterising its properties in detail, these physicists are now ready to work towards their ultimate goal: building the fabled nuclear clock. If realised, this highly accurate clock could revolutionise various technologies, including ultra-precise satellite-based navigational systems.

Next, we introduce Dr Peter Evans at the University of Queensland, whose research aims to unite quantum mechanics with cosmological theories. He argues that on quantum scales, the idea of cause and effect does not need to follow a one-way passage of time. If correct, his theories could represent a significant step forward in understanding the true nature of the universe.

On the theme of cosmology, our fifth article in this section introduces the Virgo Interferometer, based near the city of Pisa in Italy. By detecting and analysing gravitational wave signals, arising from collisions of black holes or neutron stars millions of lightyears from Earth, this machine is advancing our understanding of fundamental physics, astronomy and cosmology. In our exclusive interview, Dr Jo van den Brand discusses Virgo's achievements, plans for the future, and the fascinating field of gravitational wave astronomy.

Continuing with interferometry, in which path differences in light waves are measured as the light is split apart and recombined, we next meet Dr Stephanie Manz and Dr Thorsten Schumm at TU Vienna. By exploiting matter waves rather than light, these researchers are developing a new interferometer that promises to offer exciting experimental opportunities.

From light waves to matter waves to sound waves, our penultimate article in this edition introduces an exciting new project that is paving the way for technologies whose operation is based on sound. Combining the expertise of more than 30 scientists and engineers, the 'New Frontiers of Sound' project aims to expand the role of acoustic waves in driving technological progress.

In our final article of this exciting edition of *Scientia*, we explore a strange phenomenon that occurs for several hours after sunset, in which vast bubbles of plasma form in the upper atmosphere, before rising upwards into space. As these bubbles can disrupt radio signals that satellites use for navigation and communication, Dr Joe Huba at Syntek Technologies uses computer simulations to gain a better understanding of their behaviour. His team's work is providing researchers with a more complete understanding of Earth's atmosphere, while also providing critical insights for mitigating disruptions to our communication and GPS systems.

CERN'S FUTURE CIRCULAR COLLIDER

Geneva-based particle physics research centre, CERN, plans to build a £20bn particle accelerator that is almost four times longer than today's largest and most powerful accelerator, the Large Hadron Collider (LHC). At 100 kilometres long, this '[Future Circular Collider](#)' (FCC) will be able to accelerate particles to unprecedented speeds, leading to collisions that are 10 times more energetic than those achieved on the LHC. Measurements taken from such collisions will help scientists in solving several longstanding mysteries in physics, such as the nature of dark matter. In this exclusive interview, we speak with CERN physicist Dr Matthew McCullough, who tells us about CERN's plans for the FCC, its remarkable capabilities, and the new physics that he is most excited to explore.



How was the idea to build the FCC first conceived?

After the discovery of the Higgs boson, it became clear to the global particle physics community that a high precision Higgs factory, such as FCC-ee (an electron-positron collider), was the obvious next step if we want to understand this curious and singular particle, and a number of different communities began seriously considering this possibility.

A Higgs factory alone is not sufficient to address the full breadth of questions we have in fundamental particle physics, so an energy frontier machine that offers

broad exploration capabilities but, importantly, can also be hosted within the same infrastructure as a precision Higgs factory, such as FCC-hh (a proton-proton collider), quickly followed suit.

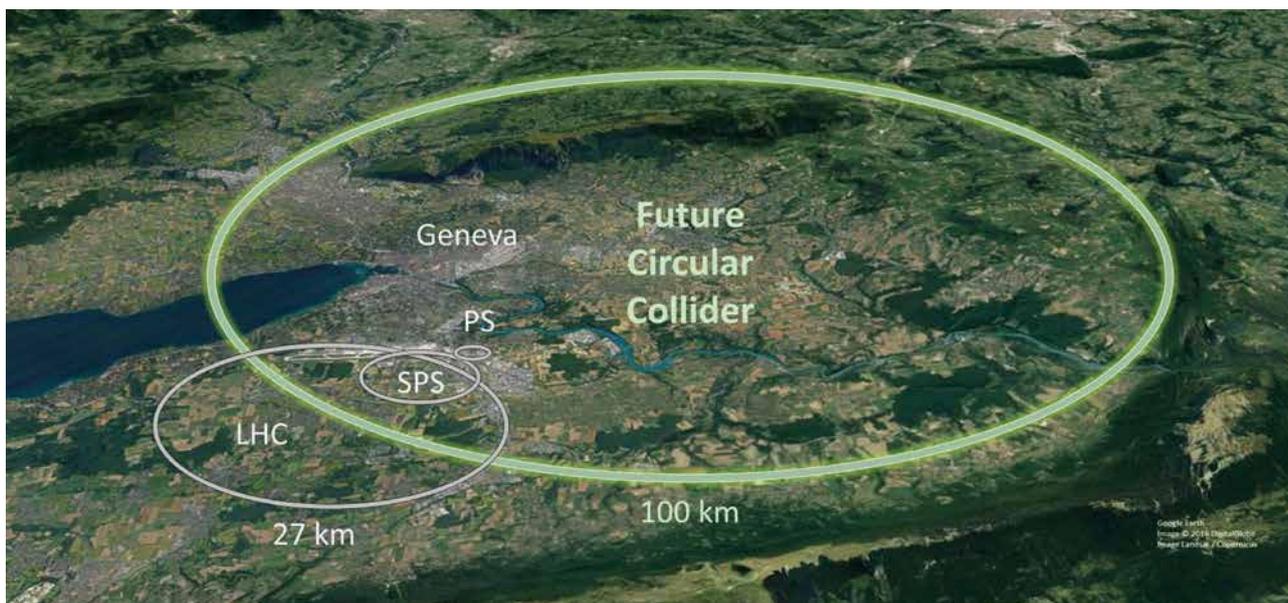
The FCC will be a whopping 100 km long – dwarfing the 27 km LHC – making it the most powerful particle accelerator in the world by far. How will the FCC's capabilities compare with those of the LHC?

The capabilities will far surpass those of the LHC, both in terms of precision and in terms of the reach to explore what exists at more microscopic distances.

For the former, let's take the Higgs boson as an example. To understand this new type of particle, it is crucial that we measure its interactions as precisely as possible. At the LHC, the best precision we can hope for is at the level of a few percent, whereas the FCC can push the precision frontier to far below the percent level, giving us unprecedented access to the world of the Higgs boson.

For the latter, the extremely high energy of FCC-hh allows us to reach the actual particles responsible for forces that are much more microscopic than the distance scales probed by the LHC. The improvement depends on the scenario,

‘The thing that excites me the most is actually very simple: it is the sheer excitement of exploring places no one has ever been before. In this case, the ‘places’ are the microscopic innards of nature which can only be explored with the FCC.’



but typically one can directly probe distance scales a factor of five smaller.

Because the FCC will be able to accelerate particles to even higher speeds, leading to higher-energy collisions, do you need to design a new class of detectors to capture previously-unattainable signals that might be created in such collisions?

Absolutely. The detectors will build on the technological advances made already at the LHC, but further innovation will be required. This is at the level of the technological hardware – for example, in designing detectors with higher resolution to track particles with greater precision.

A second aspect is the big data challenge of the FCC. The FCC-hh detectors in particular would produce enormous quantities of data to be stored, shared, and analysed. This would raise computational and big data challenges greater than we have seen before in particle physics.

However, when faced with such obstacles in the past, researchers at CERN and within the broader particle physics community have risen to the

challenge. This is, after all, how we ended up with the World Wide Web.

When do you hope construction will begin and end? What challenges do you foresee cropping up during this phase?

As a theoretical physicist I am totally unqualified to comment on construction challenges. But also, as a theorist with a long list of questions about the laws of nature to be answered, I can tell you that I hope construction begins and ends as soon as possible so that I can benefit from the knowledge the FCC will create.

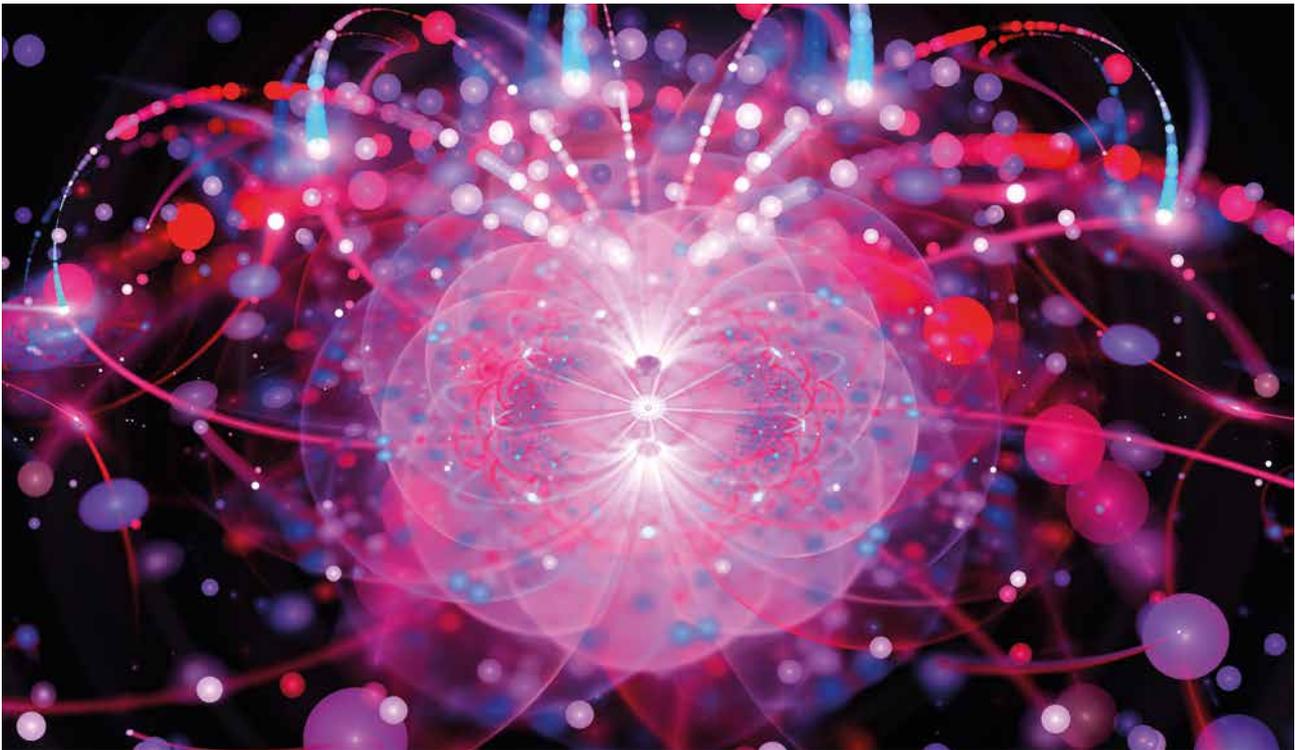
I’m particularly interested in how the FCC will be able to probe the nature of dark matter. How could collisions between normal matter particles provide information about dark matter?

Despite the fact that there is a lot more dark matter than visible matter in the Universe, we have absolutely no idea what it is. This makes the dark matter puzzle one of the most acute problems in modern physics.

In fact, we know so little about it, that the particles that make it up could still, in principle, take an enormous range of masses. Each mass range requires a dedicated experimental program to discover it. It turns out that one well-motivated mass range is around the energies available to high energy colliders such as FCC. The reason I say it is ‘well-motivated’ is because for this mass range if you have moderately-sized interactions between the dark matter and the standard model particles and you run the cosmological clock forward from early times, you typically predict the same amount of dark matter as we know exists today.

It’s sort of a Goldilocks situation, where the theory and cosmology work out to get the prediction ‘just right’. Because their mass is within range, these particles could be produced in colliders, but, being dark, we couldn’t actually detect them. However, just as with Goldilocks, some tell-tale traces of the dark matter would be left over.

For instance, we know that momentum is conserved in nature, and if dark matter is produced, it will carry away momentum that we don’t measure in the detector. Thus, we would add



everything up and the sums wouldn't match because of 'missing momentum'. Now, this is only one of the tell-tale signatures of dark matter production, but putting the full suite of possibilities together, it turns out that the FCC can probe the vast majority of models of this type through such signatures.

How might the FCC be used to figure out why the universe appears to contain hardly any antimatter, compared to matter?

If you take the Standard Model of particle physics and again run forward the cosmological clock from the early Universe to now, you don't end up with enough matter, certainly far less than we observe. Thus, there must be something beyond the Standard Model that explains where it came from.

There are many different possibilities for how this could have happened. There is one class of theories in particular where this occurred during the transition when the Higgs field gave mass to many of the particles we know. We call this the electroweak phase transition. Modifying the dynamics of the Higgs field at this time requires modified interactions and/or new particles in the Higgs sector. It turns out that, since the FCC is uniquely effective at exploring the Higgs boson, these modifications are typically big enough to be seen at the FCC. As a result, if the matter was created during the electroweak phase transition, there's a good chance we could see the new physics responsible for it with FCC.

In terms of new physics, what possibilities are you most excited about?

The thing that excites me the most is actually very simple: it is

the sheer excitement of exploring places no one has ever been before. In this case, the 'places' are the microscopic innards of nature which can only be explored with the FCC.

If forced to be more specific, there is one measurement that I think is extremely important. This whole story of the Higgs field obtaining a non-zero value everywhere and giving mass to particles has its deep origin in the potential energy contained in the Higgs field. To measure the shape of the 'Higgs potential', it turns out that we have to measure how it interacts with itself. This is predicted in the Standard Model, but it is by no means guaranteed that the Standard Model is the appropriate description in this mysterious corner of Higgs physics.

Thus, for me, this is one of the most important questions we have, central to the questions surrounding the Higgs boson and the origin of fundamental particle masses. At the LHC we can't measure the Higgs self-interactions well at all, so after the collider has finished running, we will have a very poor understanding of this core structural aspect. On the other hand, the FCC can measure this hidden corner of the Standard Model to a precision of a few percent, providing a clear window into the Higgs potential.

Finally, when the LHC was being developed, there were some concerns about existential dangers associated with conducting such high-energy experiments. Many worried about black holes being generated on Earth, and other doomsday scenarios. Are there any genuine concerns this time around?

These days we certainly do have reasons to be concerned for the future of our planet, but the FCC isn't one of them!

QUARK BINDING: SOLVING A QUANTUM ENIGMA

Quantum Chromodynamics is arguably the crowning achievement of modern particle physics – explaining the very existence of a vast majority of stable, observable matter in the universe. All the same, the theory is far from complete. **Professor Klaus Peters, Professor Miriam Fritsch and Professor Wolfgang Gradl** at three universities in Germany have dedicated their research to this intriguing field. Stemming from the very first confirmed observation of a ‘tetraquark’ in 2013, their research is opening up the door to a new generation of particle physics experiments.

The Standard Model

On the surface, the Standard Model of particle physics appears to give an elegant summary of the universe’s most fundamental particles and forces, explaining how they fit together to form larger, more complex structures. Protons, for example, are made up of three elementary particles named quarks, which are held together by the strong nuclear force. The strong nuclear force is itself mediated by massless particles called gluons.

In reality, however, the picture isn’t this simple. A wide variety of more complex processes are also at play, which mean that the actual mass of a proton is far heavier than the combined masses of its quarks.

‘It is sometimes said that the whole is more than the sum of its parts,’ says Professor Klaus Peters of Goethe University Frankfurt. ‘For the proton, this expression is literally true. The sum of the masses of its constituent quarks account for less than 2% of the proton’s total mass, with the rest resulting from the kinetic and binding energies among

quarks due to dynamics of the strong nuclear force.’ Over the past several decades, particle physicists have put immense effort into finding out more about these mysterious properties.

Successes and Failures of Quantum Chromodynamics

So far, these efforts have culminated in a highly advanced theory named Quantum Chromodynamics (QCD). As a key part of the Standard Model, QCD directly predicts the existence of hadrons – subatomic particles made up of quarks, which include baryons and mesons. Baryons, such as protons and neutrons, are made up of three quarks, while mesons are short-lived particles comprising a quark and an anti-quark. ‘QCD describes the properties of quarks and their interactions through gluons,’ explains Professor Miriam Fritsch of Ruhr University Bochum, a long-term collaborator of Klaus Peters. ‘It is very successful in predicting processes at high energies where quarks are weakly coupled together.’

Baryons and mesons may be relatively easy for physicists to study, but



according to QCD, they aren’t the only particles that can be made up of quarks. In fact, the theory predicts a diverse family of quark-based particles – many of which contain lower-energy quarks, whose properties are strongly connected with each other. However, these cases are much more difficult for QCD to deal with. ‘At low energies, quarks become far more strongly coupled together, making it hard to predict the properties of bound systems from first principles,’ says Professor



can pop into existence. Almost as soon as the $Y(4260)$ particle is created, it subsequently decays into several products, which are picked up by the detector system surrounding the original collision spot of the electron and positron beams. By analysing these decay products, the physicists can learn more about the structure of $Y(4260)$.

However, while unravelling the mysteries of $Y(4260)$, the BESIII Collaboration found something even more surprising. By analysing the decay products of the electrically-neutral $Y(4260)$ particle, they identified another electrically-charged particle, which they named $Z_c(3900)$. Under normal circumstances, $Z_c(3900)$ would appear to be a conventional meson. The decay products suggested that it contains a heavy type of quark called a 'charm' quark, along with its anti-matter counterpart, an 'anti-charm' quark.

However, a charm quark together with an anti-charm quark results in a neutral particle. In order to make a particle with electrical charge, at least two additional quarks are needed. That left only one option: $Z_c(3900)$ must be an elusive four-quark particle – an 'exotic hadron' made up of two quarks and two anti-quarks.

QCD and the quark model had already predicted these particles 60 years ago. Since 2005, a handful of candidates for four-quark particles had been observed, but each one had only been detected in a single experiment. Soon after the discovery of $Z_c(3900)$ by the BESIII experiment in 2013, it was subsequently confirmed by the Belle Collaboration in Tsukuba, Japan, and again by data from another experiment at Cornell University. This marked the first time that more than one experiment claimed to observe the same four-quark particle.

Investigating Four-Quark Particles

The discovery of the BESIII Collaboration was a triumph for particle physics – confirming long-standing theoretical predictions. 'The doubtless discovery of $Z_c(3900)$ in 2013, which cannot be explained as a conventional state in the quark model, was an important step,' says Wolfgang Gradl. 'Thus, the detection of the $Z_c(3900)$ with a minimum of four constituent

quarks/anti-quarks was one of the greatest discoveries in this decade.' Beyond the observation of $Z_c(3900)$ itself, further studies into its properties will prove to be vital for physicists to understand strongly-coupled QCD.

As Klaus Peters explains, such studies open up a rich new area of particle physics, since four-quark particles, and potentially even more exotic particles, could be composed of vast combinations of quarks and gluons. 'QCD principles allow for even more complex objects,' he says. 'Because of their large variety of possibilities, they should outnumber all the conventional particles such as baryons and mesons.' However, despite these intriguing possibilities, there is still a long way to go before such studies can take place. Before then, physicists need to learn more about the fundamental properties of exotic particles.

A New Generation of Particle Physics Experiments

At the heart of the issue is the very fact that exotic particles are so elusive. Klaus Peters says that physicists have yet to answer why they have escaped observation for so long: 'The question is: if exotic bound states are there, then why don't we see them? None of them are stable and many particles are very close together and overlapping. Therefore, they cannot be distinguished easily.' Professors Fritsch, Gradl and Peters believe that answers to the questions posed by multi-quark particles could also help to answer a much more fundamental question: unravelling the mysteries of the universe's most stable particle, the proton. 'All these points back to a simple question: how does the binding among the quarks within the proton work, and how does it generate its mass?' adds Miriam Fritsch.

As the capabilities of particle physics experiments ramp up in the coming decades, these questions will form the basis of a new era of experiments in the field. 'The proof of the existence of exotic hadrons is made and the door is opened to a new territory, but a lot of open questions remain,' says Miriam Fritsch. 'Now, it is up to a new generation of experiments to unravel the puzzle.'

A key part of this new generation of research will soon take place in Professors Peters, Fritsch and Gradl's home nation of Germany. 'The PANDA Detector is under construction at Darmstadt's Facility for Antiproton and Ion Research (FAIR), utilising an antiproton-beam for a large variety of high-statistics and high-precision measurements in hadron physics. It will begin operation in 2025,' Klaus Peters concludes.

With the help of this highly sophisticated detector system, the particle physics community could soon ascertain the internal structure of $Z_c(3900)$ in unprecedented detail. This could bring them one step closer towards unravelling the mysteries of the strongly-coupled matter described by QCD, and perhaps, understanding the true nature of the Standard Model.



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Professor Klaus Peters completed his doctoral degree in Physics at the Johannes Gutenberg University Mainz in 1991. He then worked at Bochum as a lecturer and was a visiting researcher at CERN in Geneva and SLAC in Stanford. In 2004, he became Professor at the Goethe University Frankfurt with a joint appointment at GSI Helmholtz Centre for Heavy Ion Research GmbH in Darmstadt. Among other activities, Professor Peters is member of the GlueX, BESIII, and the PANDA collaborations, and has been the spokesperson of the PANDA collaboration since 2017. His principal research interests are exotic hadron spectroscopy with light, strange and heavy quarks.

Professor Miriam Fritsch completed her doctoral degree in Physics at the Friedrich Alexander University Erlangen in 2002. She then worked at the Universities of Bochum, Karlsruhe and Mainz, and was a visiting scientist at SLAC in Stanford, before becoming Helmholtz Young Investigator Group leader in Mainz (2011–2016). In 2016, she became Professor at the Ruhr University Bochum. Among other activities, she is a member of the BaBar, BESIII and PANDA collaborations. Professor Fritsch's principal research interests are hadron spectroscopy, especially with heavy quarks, and the development of detector systems with silicon pixel sensors used in this field.

Professor Wolfgang Gradl completed his doctoral degree in Physics at the University of Heidelberg in 2001. He then worked at the Universities of Heidelberg and Edinburgh and was a visiting researcher at SLAC in Stanford, before moving to the Johannes Gutenberg University Mainz in 2008. Here, he has been working as a Professor since 2011. Among other activities, Professor Gradl was member of the Hera-B and BaBar collaborations and he has been the co-spokesperson of the BESIII collaboration in Beijing, China, since 2013. His main research interests lie in hadron spectroscopy and Standard Model tests using particles containing charm and bottom quarks.

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FUNDING

DFG – SFB 1044
DFG – FG 2359
DFG Cluster of Excellence Prisma Mainz
BESIIICGEM H2020-MSCA-RISE-2018
GSI Helmholtz Centre for Heavy Ion
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THE THORIUM ISOMER: PAVING THE WAY FOR NUCLEAR CLOCKS

Atomic clocks have long been the most accurate timekeeping devices known to physics, but thanks to research carried out in recent years, it looks like their reign could soon be over. As part of the European consortium ‘nuClock’ (nuclock.eu), **Dr Peter Thirolf**, **Dr Lars von der Wense** and **Benedict Seiferle** at Ludwig-Maximilians University Munich are working towards building the fabled, even more precise nuclear clock, through investigating the nucleus of Thorium-229. If their clock is realised, the researchers’ work could soon see strides towards applications ranging from ultra-precise GPS, to new, rigorous tests of the most fundamental constants of physics.

Keeping Time

From grandfather clocks to digital watches, the timekeeping devices we all rely on are united by a need to accurately measure the frequency of an oscillating system known as a ‘frequency standard’. While more traditional grandfather clocks, for example, keep track of time by continually measuring the frequency of a swinging pendulum, conventional digital watches do so by measuring the regular pulse of a quartz crystal with an electrical current passing through it.

However, as any physicist will tell you, it is impossible for any measurement device to be completely accurate. Over time, even the slightest errors in a clock’s frequency standard will stack up, making the device increasingly unreliable – a serious issue for physicists carrying out meticulously precise experiments.

In the 1930s, US physicist Isidor Isaac Rabi proposed a frequency standard that would make inaccurate clocks a problem of the past. Named the

‘atomic clock’, Rabi’s device operated by measuring the frequencies of microwave signals emitted by the electrons of atoms as they jumped between different orbits, or ‘energy levels’. With modern versions of atomic clocks, physicists can now measure time within an error of just one second every 30 billion years, far more than the age of the Universe. However, there are applications involving time measurements where even this barely perceptible margin of error is not small enough.

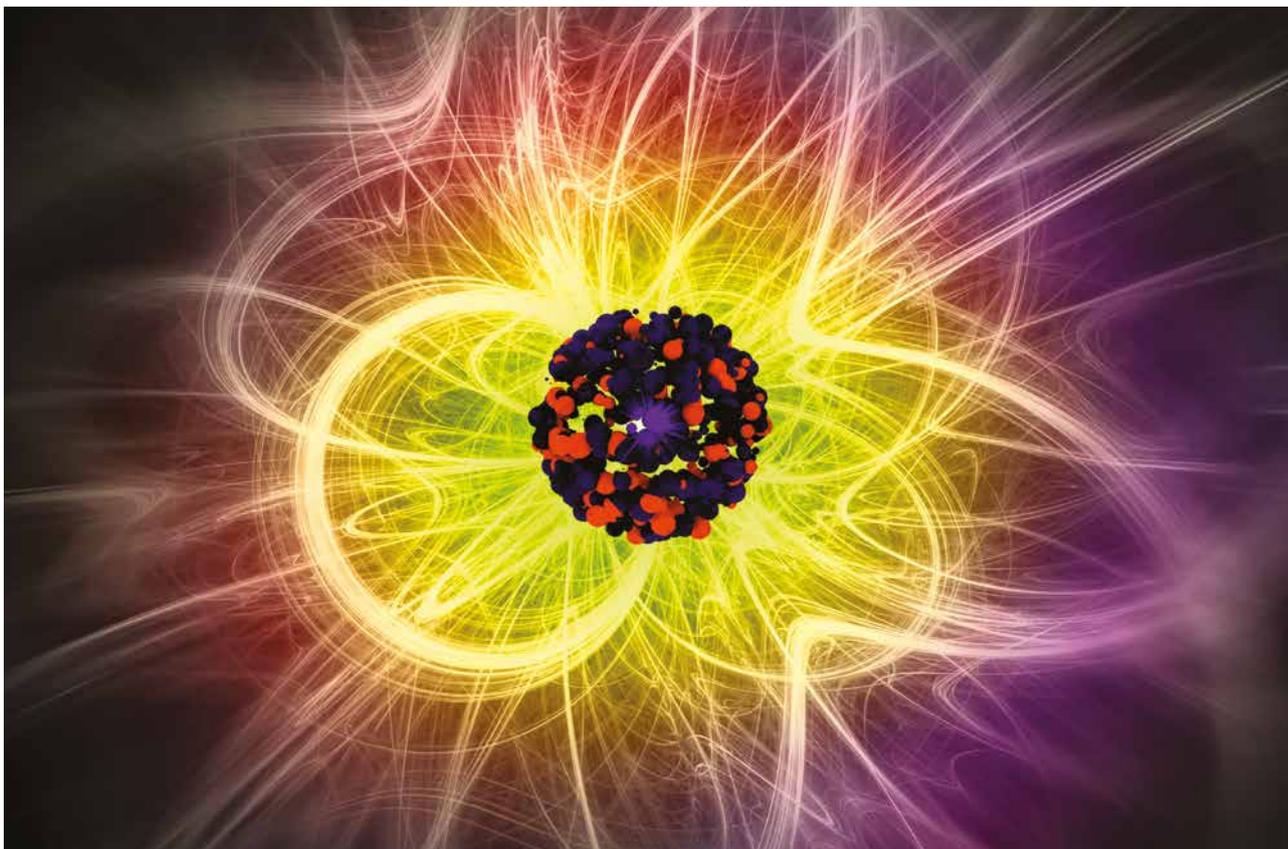
Enter the Nuclear Clock

Intrinsically, the margins of error required by some envisaged applications aren’t possible with even the most accurate atomic clocks. Instead, a new generation of clock is needed, using the frequencies given off by atomic nuclei as they transition between energy levels as their standard. ‘Today’s most precise time and frequency measurements are performed with optical atomic clocks,’ explains Dr Peter Thirolf, of Ludwig-Maximilians University Munich (LMU). ‘However, it has been proposed that



they could potentially be outperformed by a nuclear clock, which employs a nuclear transition instead of an electron transition.’

These transitions between nuclear energy levels are analogous to those between electron energy levels. They may also stay for a period of time in a specific energy level before this so-called ‘isomer’ will relax back into the lowest energy level of the nucleus (the ground state). The nucleus of an atom



is 10000–100000 times smaller than the atom itself and is thus less prone to external perturbations.

Together, these properties mean that the margins of error of the frequencies given off by nuclei during a transition can be lower than those of an electron transition, making nuclear transitions a potentially even more accurate frequency standard for timekeeping devices. So, with such clear advantages, it might come as a surprise that not a single nuclear clock has yet been built.

The Elusive Thorium Isomer

At the heart of the issue is the fact that compared with atomic electrons, it is far more difficult to force nuclei into higher (or ‘excited’) energy levels artificially. This is because the excited energy levels of nuclei typically have far higher energies than those of electrons. Electrons can be ‘excited’ into higher energy levels by shining laser light of particular energies on them. However, even today’s most cutting-edge narrow-bandwidth laser technology cannot create light with energies high

enough to force transitions to typical nuclear energy levels, which means that practically all presently known nuclear energy levels are currently out of reach.

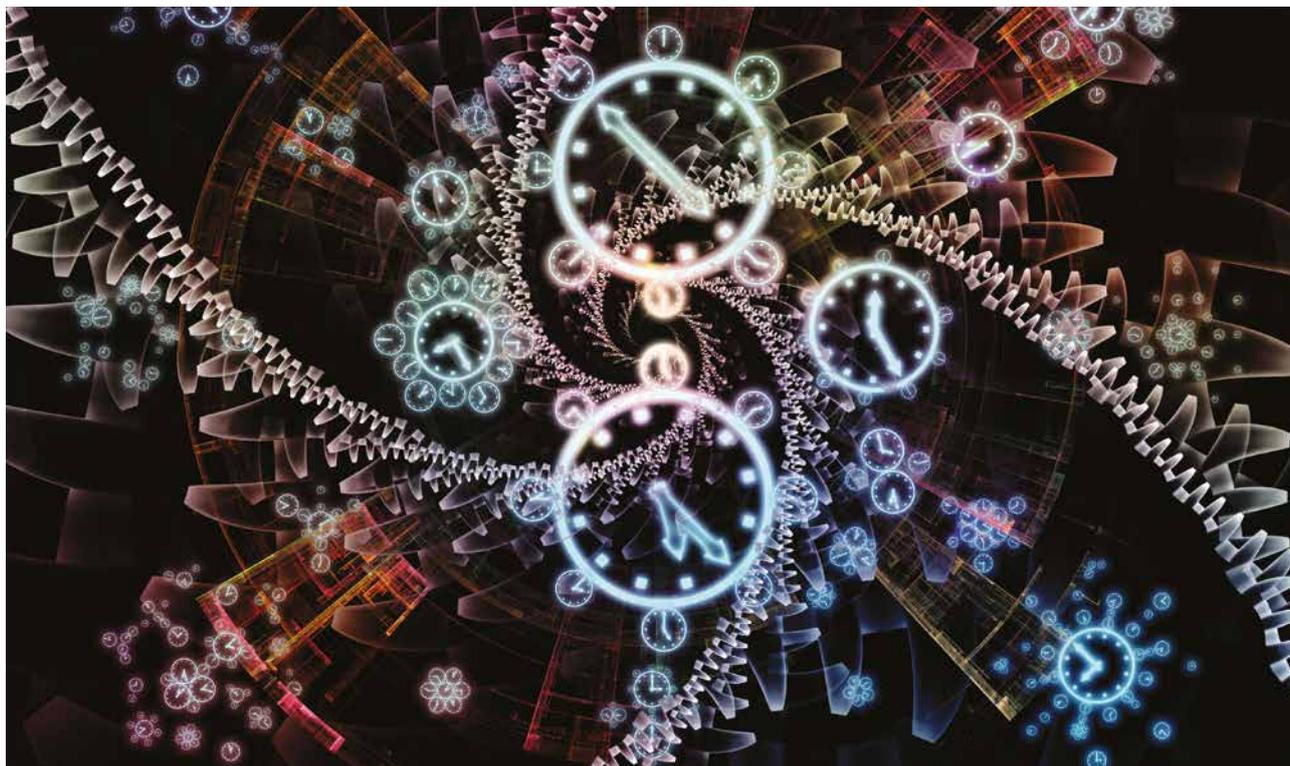
However, there is a unique exception. There is only one known nuclear energy level that could serve as a nuclear clock using currently available technology, namely, the first excited level of Thorium-229, with a predicted lifetime of a few thousand seconds. This excited energy level of Thorium-229 is often called the thorium isomer.

Consisting of 90 protons and 139 neutrons, the thorium isomer is ideally suited to serve as an ultra-precise and stable nuclear frequency standard, due to its long lifetime and the low energy required to access this energy level (called the ‘excitation energy’). Having predicted these properties through decades of theoretical studies, many physicists have attempted to observe direct transitions between the thorium isomer and the ground state of Thorium-229. However, despite several decades of research, none have been able to do it.

An Idea Confined to Theory

The previous inability of researchers to observe the thorium isomer directly is not for a lack of trying. In fact, for 40 years, nuclear physicists have tried to identify and characterise the elusive transition from the thorium isomer down to the lowest energy level of thorium-229. Until recently, evidence for the thorium isomer’s existence could only be inferred from indirect measurements, which suggested an extraordinarily low excitation energy of 7.8 ± 0.5 electronvolts. Thus, the thorium isomer represents the lowest nuclear excited level reported so far.

Electronvolts are a commonly-used unit in nuclear physics, describing the amount of energy gained by an electron after moving across an electric potential difference of one volt. In comparison to the thorium isomer’s excitation energy of 7.8 ± 0.5 electronvolts, most nuclei require millions of electronvolts to force them into higher energy levels, making the thorium isomer an extremely enticing prospect to physicists. Dr Thierolf and his colleagues, Dr Lars von



der Wense and Benedict Seiferle, embarked on a mission to overcome the difficulties faced by physicists in the past to detect the transition experimentally for the first time.

Exploring an Elusive Transition

In a 2016 study, the LMU team, together with colleagues from Mainz and Darmstadt, achieved the first ever experimental detection of a direct transition between the thorium isomer and the ground state of Thorium-229. Building upon decades of previous work, the team achieved this through observing a specific decay signature. Completing a search by nuclear physicists that was conducted worldwide for about 40 years, they recently succeeded in realising the first direct detection of this nuclear energy level through its decay via a transfer of the thorium isomer's nuclear excitation energy to an electron. This electron is then expelled from the thorium atom and detected.

Having observed this transition for the first time, the physicists could now explore it in more detail. Since the nucleus of Thorium-229 is unstable, one of the first properties they looked at was the time it takes for half of the thorium isomers in a system to relax back into the ground state. This property is known as the 'half-life'. The initial work laid the foundation for precise studies of the thorium isomer's decay parameters and subsequently, the first measurement of the half-life of the neutral isomer was achieved.

After these studies, the unique splitting of energy levels found in the thorium isomer was explored, known as its 'hyperfine structure'. Soon after, in collaboration with laser experts from the German National Metrology Institute and colleagues

from Mainz, collinear laser spectroscopy was applied to the team's experimental setup to obtain the hyperfine structure of the thorium isomer, which provided detailed information about nuclear properties. Having experimentally observed the thorium isomer for the first time, and after exploring its properties in detail, the physicists are now ready to work towards their ultimate goal: the nuclear clock.

A Transformation of Timekeeping

The numerous recent discoveries around the thorium isomer have made precise, ultra-stable nuclear clocks look like a real possibility in the near future. Significant insight into the properties of the thorium isomer's elusive nuclear energy level have been achieved in the last few years, paving the way towards laser-based control of the thorium isomer. Thus, the ultimate goal of developing an ultra-precise nuclear frequency standard, the nuclear clock, could be realised. If so, this new degree of precision would reduce uncertainties in timekeeping devices to minuscule levels. In addition, fundamental physical constants could soon be subjected to the most rigorous tests ever performed on them.

A nuclear clock promises a lot of intriguing applications in applied as well as fundamental areas of physics, ranging from an improved precision of satellite-based navigational systems (such as GPS) and seismology (monitoring seismic activity with high precision using a nuclear clock as a gravity sensor) to investigating possible time variations of fundamental physical constants. In the next few years, physicists will work towards making the first ever nuclear clock a reality.



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Dr Peter Thierolf obtained his PhD from the University of Heidelberg in 1992. After postdoctoral research at the Max-Planck-Institute for Nuclear Physics in Heidelberg and the National Superconductor Cyclotron Laboratory at Michigan State University in the USA, he joined Ludwig-Maximilians-University Munich, where he became lecturer after his habilitation in 2004. Dr Thierolf's research interests include investigating the structure of exotic nuclei, instrumentation for medical physics applications, nuclear mass spectrometry, laser ion acceleration and fundamental physics.

Benedict Seiferle studied Physics at Ludwig-Maximilians-University Munich where he earned his master's degree focusing on the direct detection of the Th-229 isomer. At present, Seiferle is working on his PhD thesis, which aims for a direct and precise characterisation of the properties of Th-229m. During his work he already succeeded in measuring the isomer's lifetime and is currently proceeding towards a direct measurement of the excitation energy.

Lars von der Wense received his scientific education in physics and mathematics at the University of Hamburg. He earned his diploma in physics with a topic in string theory before moving to the University of Cambridge, UK, for a Master's course in Applied Mathematics. For his PhD thesis he changed fields to experimental physics and has been working on the Thorium-229 project at Ludwig-Maximilians-University Munich since 2011. He received his PhD in 2017 for the first direct detection of 229mTh. This result was elected by the editors of Physics World as one of the Top 10 Physics Breakthroughs of 2016. Currently he is continuing his research on Thorium-229 as a postdoctoral researcher.

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FUNDING

European Union (Horizon 2020: FET-OPEN)
Deutsche Forschungsgemeinschaft (DFG)



RETRO-CAUSALITY: UNRAVELLING THE MYSTERIES OF QUANTUM COSMOLOGY

Despite many years of research aiming to unite quantum mechanics with cosmological theories, researchers in fields across physics and philosophy remain in disagreement about a solution. Now, **Dr Peter Evans** at the University of Queensland sheds new light on the debate. He argues that on quantum scales, the idea of cause and effect does not need to follow the one-way passage of time, as we understand it. If correct, his theories could dispel some of the most puzzling mysteries of quantum theory – a significant step forward in understanding the true nature of the universe.

Quantum Cosmology

For decades, scientists and philosophers alike have struggled to reconcile our current understanding of the nature of the universe with the theory of quantum mechanics. This broad field, known as ‘quantum cosmology’, encompasses a wide variety of efforts to unite quantum behaviours, which unfold on the very smallest of scales, with processes such as the universe’s accelerating expansion.

Such a goal is a mammoth undertaking. Despite the fact that our current theories of quantum mechanics and cosmology each work well on their own, they still appear to be completely incompatible with each other. So far, no one has come close to merging them into a single theory.

Dr Peter Evans at the University of Queensland considers a different angle to the problem: what if events that happened in the past could have been caused by events in their futures? The idea is clearly incompatible with our

current idea of spacetime, in which time progresses in one direction.

However, Dr Evans argues that given a conceptual framework built from the right background assumptions, his ideas could answer some of the most pressing questions posed by quantum cosmology. To justify these claims, he has drawn together a variety of concepts first devised in previous studies, in fields including cosmology, quantum mechanics and philosophy.

Redefining the Cause and Effect Chain

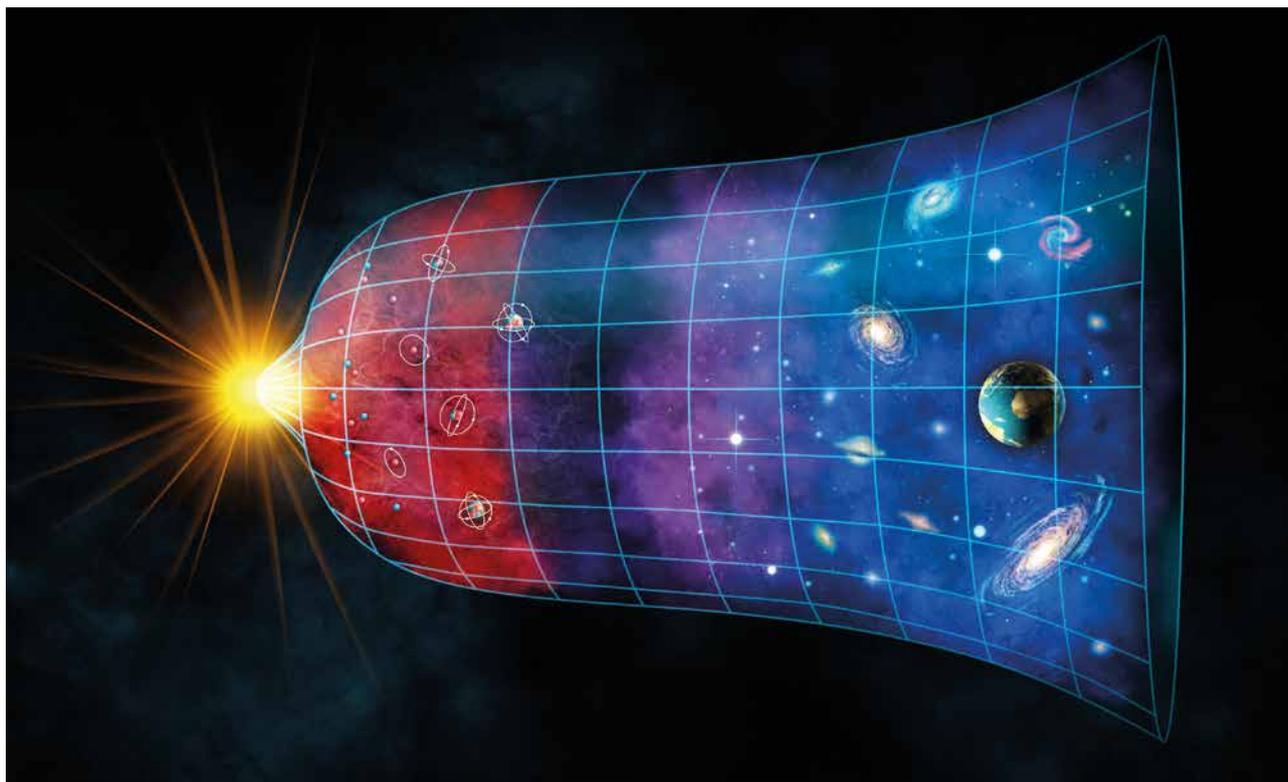
Philosophers have incorporated the idea of cause and effect into their arguments for many centuries – many of them using it to justify their beliefs about the origins of the universe. The concept describes how an event cannot happen unless it has been triggered by another event, which happened in its past. Today, the concept of cause and effect continues to be important in quantum mechanics, where it has been given the name ‘causality’. In this context, the idea demands that even on quantum scales, one event must always have been caused by another.



Contrary to well-established philosophical theories, Dr Evans argues that in quantum mechanics, chains of events do not necessarily need to play out within our limited, one-directional view of the flow of time. Where conventional physics experiments ultimately rely on this more conventional concept, his work is based on the possibility of backwards-in-time, or ‘retro’-causality, where quantum mechanics allows for the occurrence of an event that has been triggered by another event occurring in its future (from our perspective).

Many researchers continue to discredit retro-causality as a flawed idea, since many scientific theories are fundamentally based around the idea that time is one-directional, and cannot

‘My research considers the possibility of retro-causal influences playing a role in solving some of the mysteries of quantum theory’



flow backwards. If retro-causality did turn out to be true, they would argue that many of the fundamental laws of the universe as we currently understand it would need to be completely re-written. However, Dr Evans has set out to prove that retro-causal influences are not only possible, but could also provide a variety of meaningful solutions to the challenges faced by researchers of quantum cosmology.

Considering Retro-Causal Influences

One of the biggest puzzles currently faced by quantum theorists is the undeniable observation of ‘action at a distance’ interactions, where certain events must have been triggered by others happening simultaneously. As Einstein clearly showed, this shouldn’t be allowed to happen, since the universe has a fundamental speed limit – the speed of light – which must mean that an event can’t happen at the same time as the event it has been caused by.

In addition, quantum theory appears to suggest that objects on quantum

scales can only be ‘real’ when they are observed; otherwise, they only exist as a cloud of potential positions in space and time. Many theorists argue that this blurry idea of reality can’t really represent what is actually happening, and that it is simply unscientific to say that an object doesn’t exist simply because it isn’t being measured.

As Dr Evans explains, these types of long-standing problems could be solved if quantum mechanics allowed the chain of cause and effect, which underlies the behaviour of the universe, to be not restricted to a one-way flow of time. ‘My research considers the possibility of retro-causal influences playing a role in solving some of the mysteries of quantum theory,’ he says. ‘Some of these quantum peculiarities, such as apparent action at a distance or the definite reality of the quantum system between measurements, obtain a natural and intuitive interpretation when considered as arising as a result of retro-causal influences at the quantum scale.’ Dr Evans believes that if certain perhaps unorthodox background

assumptions are made when stating the nature of the universe, there is nothing to say that retro-causality isn’t possible.

Conceptual Framework for Retro-Causality

The first of these unorthodox background assumptions is called the ‘block universe’ model, which states that the universe exists as an unchanging four-dimensional block. Four-dimensional spacetime is a widely used concept amongst cosmologists, describing how the three-dimensional space in which we exist is continually changed by the fourth dimension, which we know as time. Recently, some theorists have argued that if the universe exists as an unchanging four-dimensional block, time must not be some irreversible concept; rather, everything that will ever happen is essentially happening simultaneously. Within this framework, retro-causal influences may be allowed to occur from our perspective.



The second assumption is named the ‘interventionist account of causation’, which describes how certain events can be caused by other events, but only if the variable responsible for the first event was changed in a certain way. This is in contrast to the conventional idea that all events must have been triggered by past events to which they are linked, no matter the nature of the variable change that gave rise to the first event. If connections between events really are more exclusive, retro-causal influences could in fact become a necessary property of the nature of the universe.

To adopt each of these ideas, Dr Evans argues that we would need to let go of our current view of the past as something we can know everything about. Instead, he says, we should adopt a more flexible idea of time. If these background assumptions are made, he believes that retro-causality can be seen as a feasible solution to many of the problems posed by quantum cosmology. ‘The notion of retro-causality cannot be ruled out on analytic grounds, and so comprises a viable conceptual framework for attempting to understand quantum phenomena,’ he explains.

Agent-Relative Causality

Having established this groundwork, Dr Evans then aimed to describe the conditions in which retro-causal events would occur. He has concluded that in order for his ideas to work, a highly unorthodox piece of philosophy is needed: we would need to view causality as an ‘agent-relative’ idea.

In this context, an ‘agent’ is a causal actor in the world, which we certainly take humans to be. We would probably take certain advanced robots, and perhaps even intelligent extra-terrestrial lifeforms, to be agents also. Viewing causality as an ‘agent-relative’ notion is counterpoised to the idea that causality is an objective feature of the world – out there independently of the causal players in the world, and existing even if there were no humans. Agent-relative causality implies that there is some key ingredient to the way that agents interact with the world that is integral to what we think causality is fundamentally.

By extending this notion to quantum causality, Dr Evans claims that some of the mysterious behaviours of quantum systems would begin to look like a symptom of the agent-relative nature of causality, and not as some ad hoc injection of the role of the agent in quantum mechanics, as one finds in the measurement problem.

‘Causality can be understood as an agent-relative notion, thereby highlighting the fact that the agent is able to play a significant part in the interpretation of quantum theory, without the postulation of any extra agent-centric phenomena,’ Dr Evans describes. ‘That is, we don’t need to specify any special new rules that agents interacting with quantum systems need to obey; it’s the fundamental causal rules that agents necessarily obey that bring about the peculiar quantum behaviour.’

If this idea is correct, the task of researchers studying the nature of causality would become far easier. Ultimately, it could break down the mystery of processes including action at a distance, and the reality of quantum objects when they are not being observed.

A New Take on Quantum Cosmology

Quantum cosmology has now become one of the most hotly debated fields among both physicists and philosophers, with very little agreement being reached amongst researchers over the very nature of our reality. In this stagnant academic environment, the approach taken by Dr Evans could prove to move the discussion along from its current deadlock – dispelling the idea that quantum observations are not consistent with our current understanding of causality.

Ultimately, this could allow for important new insights into the nature of the universe, bringing researchers one crucial step closer to reconciling quantum mechanics with the most fundamental theories of cosmology.



Meet the researcher

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Dr Peter Evans was awarded his PhD from the University of Sydney in 2011, for a thesis entitled *A Study of Time in Modern Physics*. After graduating, Dr Evans joined the University of Queensland in 2014, where he now works as a Discovery Early Career Research Fellow of the Australian Research Council (ARC), pursuing the long-term task of ‘a philosophical exploration of simulating and controlling the quantum world’. His main research interests include philosophy of physics and science, quantum foundations, and metaphysics. He has already achieved several prestigious awards to pursue his work, including the ARC Discovery Early Career Researcher Award, which he received in 2017.

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FUNDING

Australian Research Council (ARC)

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AUSTRALIA

THE VIRGO INTERFEROMETER

Located near the city of Pisa in Italy, the Virgo interferometer is the most sensitive gravitational wave detector in Europe. The latest version of the interferometer – the Advanced Virgo – was built in 2012, and has been operational since 2017. Virgo is part of a scientific collaboration of more than 100 institutes from 10 European countries. By detecting and analysing gravitational wave signals, which arise from collisions of black holes or neutron stars millions of lightyears away, Virgo's goal is to advance our understanding of fundamental physics, astronomy and cosmology. In this exclusive interview, we speak with the spokesperson of the Virgo Collaboration, **Dr Jo van den Brand**, who discusses Virgo's achievements, plans for the future, and the fascinating field of gravitational wave astronomy.



CREDIT: EGO/Virgo

How are observable gravitational waves generated?

Observable gravitational waves are generated by massive compact objects, such as neutron stars and black holes, that experience extreme accelerations. Since gravitational waves are perturbations in the fabric of spacetime, they affect the trajectories of light waves, and this can be detected by measuring the proper distance between the mirrors that make up the Virgo interferometer.

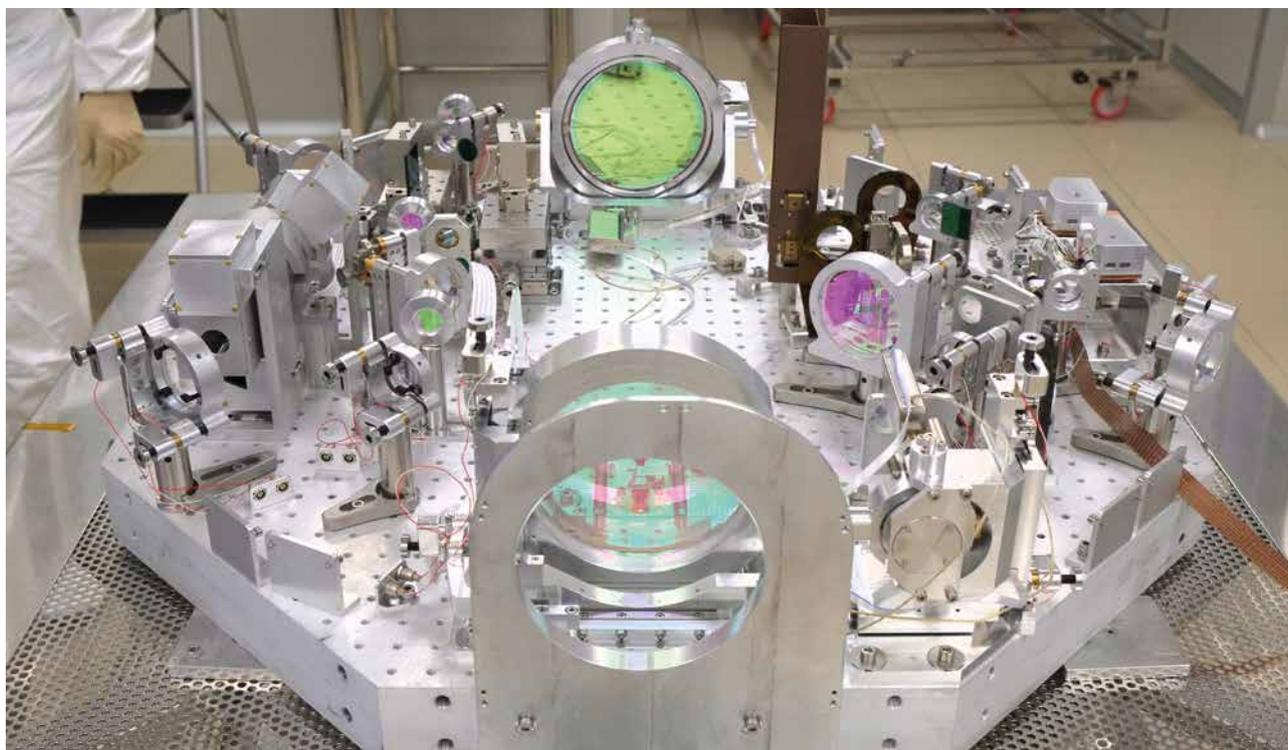
The curvature fluctuations are tiny and cause minor relative length differences. These length differences are similar in size to the ratio of the thickness of a human hair compared to the distance between Earth and the nearest star, Proxima Centauri. For this reason, it has taken decades until we succeeded to make a detection with our kilometre scale interferometers.

In February 2016, alongside LIGO, the Virgo Collaboration announced the first direct observation of gravitational waves, made using the Advanced LIGO detectors. Please tell us about the excitement amongst members of Collaboration, and what this discovery meant for Virgo.

The discovery of gravitational waves from the merger of two black holes was a great achievement and caused excitement to almost all impassioned scientists. The merger was the most powerful event ever detected and could only be observed with gravitational waves. We showed once and for all that spacetime is a dynamical quantity, and we provided the first direct evidence for the existence of black holes.

Moreover, we detected the collision and subsequent coalescence of two black holes with unexpectedly high mass, and we could test Einstein's theory of gravity, general relativity, in a regime of extreme gravity. Members of the Virgo Collaboration contributed to the data analysis and interpretation, while at the same time the work on the Advanced Virgo detector continued with a lot of dedication and intensity.

‘Observable gravitational waves are generated by massive compact objects, such as neutron stars and black holes, that experience extreme accelerations. Since gravitational waves are perturbations in the fabric of spacetime, they affect the trajectories of light waves, and this can be detected by measuring the proper distance between the mirrors that make up the Virgo interferometer.’



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What observations of gravitational waves have been made by the Virgo Interferometer itself, since this initial discovery four years ago?

While the Advanced Virgo detector did not join the first science observation run, O1, it did join runs O2 and O3. The data of O1 and O2 have been analysed, published, and the data and analysis tools have been made available to the general public. In total, we detected 11 events and Virgo contributed to five of these events, even though Virgo only joined one month out of a total of 14 months of observations in O1 and O2.

All these events originated from the merger of two black holes, except for event GW170817, detected on August 17, 2017, hence its name. Virgo was instrumental in the localisation of what turned out to be a binary neutron star merger. GW170817 saw gravitational waves in coincidence with a gamma-ray burst that was detected by the Fermi

and INTEGRAL spacecraft. The event was localised in galaxy NGC 4993 and has been studied by astronomers in wavelengths from radio to X-rays. This detection marks the birth of multi-messenger astronomy with gravitational waves and has made an enormous scientific impact.

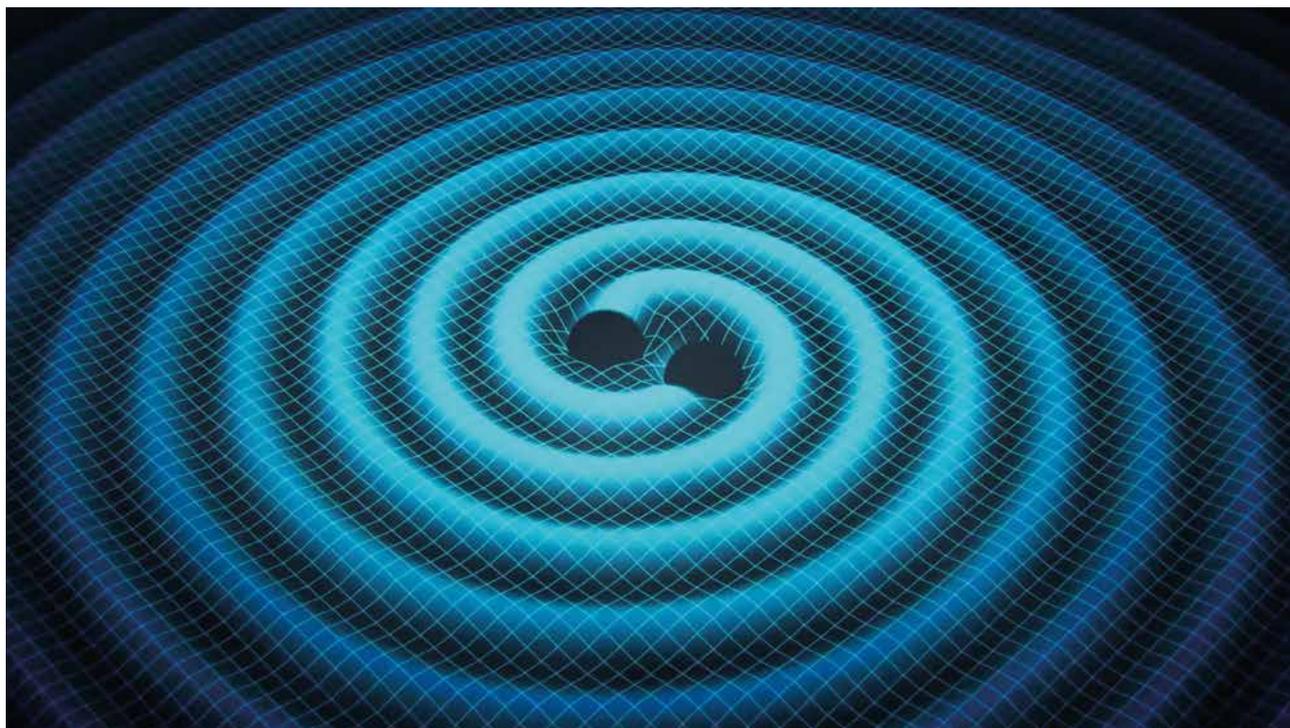
On March 27, 2020, the LIGO Virgo Collaboration suspended run O3 due to the COVID-19 pandemic in order to protect the staff at the observatories. This run was a great success, and due to the improved sensitivity of the instruments no less than 56 open non-retracted alerts were released to the public. So far, we published on one of these events, GW190425, which is consistent with being a binary neutron star merger, the second one after GW170817. At present, the collaboration is working hard on the analysis of a great scientific harvest of exciting O3 data.

In terms of physics and cosmology, what new insights have Virgo's observations offered so far?

The black hole merger observations revealed a new population of black holes with mass significantly higher than expected for stellar mass black holes. Detailed analysis demonstrated that solutions of the Einstein field equation correctly describe the observations. Together with the binary neutron star event, we demonstrated that important cosmological information can be obtained.

Moreover, the neutron star merger allowed us to extract a property known as the tidal deformability, which provides important information on the equation of state of neutron stars. It is important to note that the accuracy of such information will rapidly improve in the next observation runs when the sensitivity of the instruments improve and the event rate increases.

‘Virgo was instrumental in the localisation of what turned out to be a binary neutron star merger. This detection marks the birth of multi-messenger astronomy with gravitational waves and has made an enormous scientific impact.’



CREDIT: EGO/Virgo

The joint measurements from both LIGO and Virgo allowed us to constrain the polarisation degrees of freedom of gravitational waves. Moreover, the three-fold LIGO Virgo coincidence measurements featured a significantly improved sky localisation, allowing astronomers to more easily identify the source of an event and to look for electromagnetic counterparts.

What are you most excited about for the future of Virgo, and gravitational wave astronomy in general?

Gravitation is the least understood fundamental interaction. In an attempt to answer the many open questions, worldwide intellectual activity is ongoing, both on the theoretical front by studying the boundaries between general relativity, quantum field theory, and cosmology, and through experimental activities in astronomy, particle physics, and dark matter searches.

Gravitational wave science is a new approach that has enormous scientific potential. It would be most exciting to shed light on the important issue of the nature of dark matter, for example by observing gravitational waves from primordial black holes, or to discover signals from quantum gravity, perhaps by observing echoes in black hole mergers.

Third generation instruments such as Einstein Telescope can use signals from binary mergers to study the equation of state of dark energy. Most exciting is the realisation that the entire

Universe has been transparent for gravitational waves, all the way back to the Big Bang, and it would be wonderful to receive direct signals through this new window from our Universe at times as early as 10^{-34} seconds.

In future, how important is Virgo’s continued collaboration with other gravitational wave observatories, as well as groups operating telescopes?

Continuously improving the sensitivity of Virgo and future observation with LIGO, KAGRA and LIGO-India will be paramount, as the operation of a global international network of gravitational wave observatories (termed IGWN) will produce the best possible scientific data.

As GW170817 has demonstrated, the deepest insights will be obtained by multi-messenger astronomy and it would be spectacular if in the not too far future joint signals could be obtained from gravitational waves, electromagnetic radiation from radio to X-ray and gamma rays, neutrinos and perhaps other elementary particles.

www.virgo-gw.eu



iWave: A NEW SCHEME FOR MATTER WAVE INTERFEROMETRY

By precisely measuring path differences in light waves as they are split apart and recombined, interferometers have allowed physicists to make some of their most profound discoveries: from disproving the ether theory in the late 19th century, to the first detections of gravitational waves in 2016. Now, **Dr Stephanie Manz** and **Dr Thorsten Schumm** at TU Vienna aim to push the capabilities of interferometers further with iWave: an instrument that exploits particle-wave-duality, one of the fundamental principles of quantum mechanics. By replacing light waves with matter waves, the duo and their team believe that their new interferometer could bring about exciting experimental opportunities.



Interferometry

Interferometers are incredibly powerful tools in physics. They operate by first splitting a coherent beam of light along two paths, and then recombining them. If the conditions along the two paths are identical, then the peaks and troughs of these light waves will continue to line up, as they did the moment they were split. As they recombine, these waves are said to be 'in phase' or 'out of phase' with each other, and will constructively or destructively interfere

depending on their relative phase, while the total intensity of the original wave is conserved.

The relative phase depends on the variations of the conditions they may experience along each path – for reasons ranging from differences in the materials they travel through, to gravitational waves passing through them.

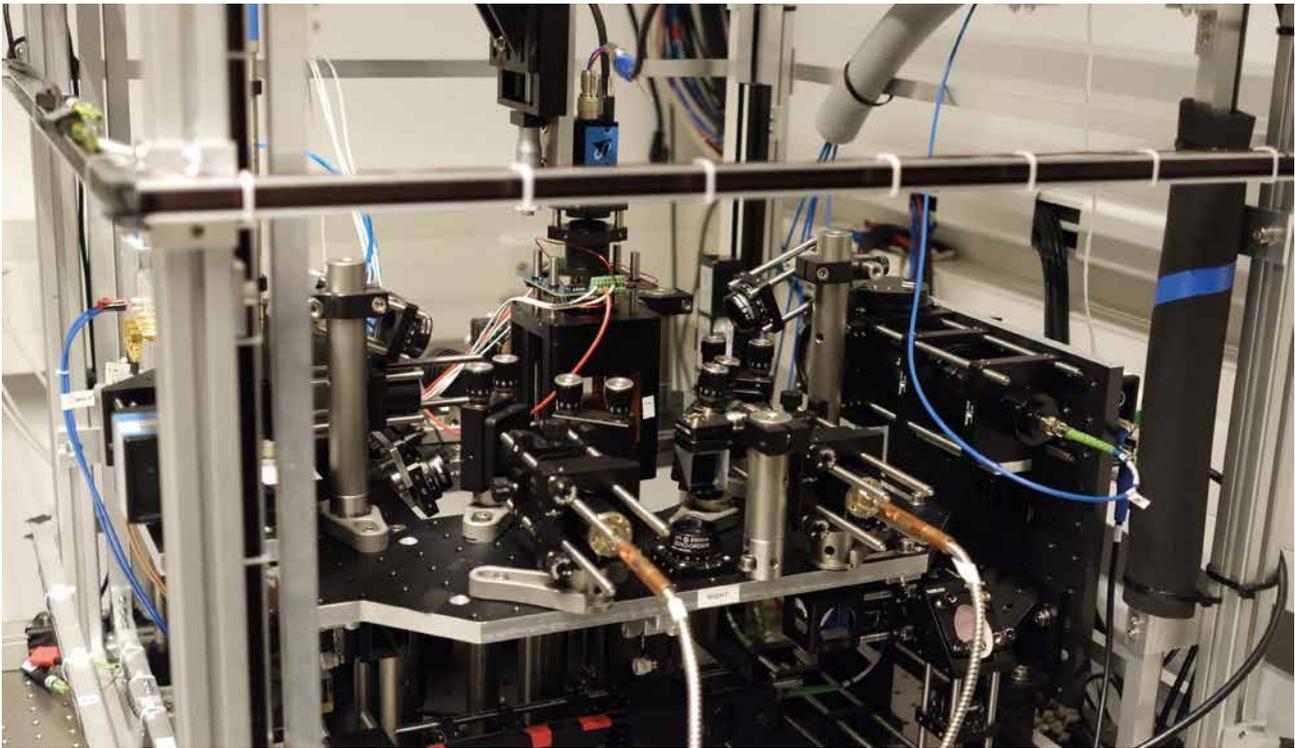
On recombination, therefore, they will interfere with each other to varying

degrees, depending on how out of phase they are. By measuring the extent to which recombined waves are modified compared to the original wave, researchers can precisely measure the extent to which the phases of each beam have been shifted.

So far, this technique has been used for purposes ranging from measurements of optical components, to detections of gravitational waves originating from black hole mergers. However, Dr Stephanie Manz and Dr Thorsten Schumm at TU Vienna believe that interferometers are still a long way from fulfilling their potential.

Beyond Photonic Interferometry

As physicists began to discover around the turn of the 20th century, the description of light as a wave cannot explain all of its observed properties. In order to account for these phenomena, researchers including Einstein proposed that it must also exist in the form of massless particles, now known as 'photons'.



At the same time, this theory suggested that massive particles – and even composite particles such as atoms – must also have wave-like properties. In perhaps the most famous example, the electron double slit experiment gives clear evidence that the diffraction patterns produced by single electrons can interfere with each other: a strictly wave-like trait. Such properties are characterised by particle ‘wavefunctions’, which describe the probability of a particle being found in a particular position when observed.

In their earlier research, published in [2005](#) and [2013](#), Dr Schumm and colleagues created the key elements of an interferometer in which light beams could be replaced with matter waves. Just like light waves, they demonstrated, particle wavefunctions should also be able to split and recombine. In this case, a phase difference in the recombining wavefunctions could be converted into a number difference in the ‘double-well’ potentials trapping the atoms – essentially moveable W-shaped containers with magnetic field walls. Ultimately, this meant that phase differences could be easily read out.

Since massive particles are extremely sensitive to forces acting on them on atomic scales, the researchers concluded that this technique would make matter wave interferometers an order of magnitude more sensitive than their traditional optical counterparts.

As Dr Manz describes, there is a key further distinction, relating to the controllability of matter wave interferometers. ‘There is a fundamental difference between photon and atom optics,’ she says. ‘While photons do not interact, atom-atom interactions lead to an intrinsic non-linearity in the matter-wave dynamics. As these interactions can in principle be controlled, this adds a powerful degree of freedom to explore new physics regimes, fundamentally inaccessible to photon optics.’

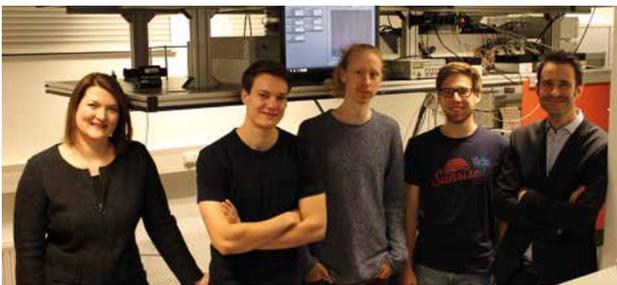
Enlisting Bose-Einstein Condensate Sources

The first hurdle that Drs Manz and Schumm would need to overcome in realising matter wave interferometry would be the fact that compared to photons, massive particles are affected by gravity – just as a bullet speeding across a field must eventually hit the ground. While ‘ballistic’ interferometers,

in which the motions of massive atoms have a vertical component, have been very [successful over the last 20 years](#), their operation time is severely limited by factors including the size of the device, and the thermal expansion of the atomic clouds.

As an alternative approach, the duo proposes the use of trapped ‘Bose-Einstein condensates’ (BECs), which are ultracold gases of atoms that mostly have the same quantum properties, in close analogy to a photon laser.

BECs are remarkably useful in physics, since the wavefunctions of individual atoms can be trapped or confined in free space using optical or magnetic fields, making them measurable on macroscopic scales. For Drs Manz and Schumm, this means that keeping the atoms trapped as compared to experiments in free fall, allows for far longer operation times. Furthermore, by deforming the potentials used to confine the atoms, the researchers could split and recombine their wavefunctions with high degrees of control, finally realising a matter wave interferometer.



Studies of this technique have dominated the team's latest research. 'Our group and others are working towards understanding how the physical properties of ultracold quantum gases have to be prepared and controlled in order to enhance their metrological gain,' Dr Schumm explains. 'The aim of this project is to establish matter-wave optics with tuneable atom interactions to realise a new class of experiments that go beyond the photon analogy.'

Problems with Phase Diffusion

Despite the numerous advantages, Dr Schumm and his colleagues identified a problem with the use of BECs in their [earlier research](#), which arises from the interactions of the atoms among themselves. Although the initial conditions of the gases could be precisely tuned, the researchers had very little control over how its individual atoms behaved during experiments, most importantly during splitting and recombining. 'The overarching problem with current BEC interferometers is that they are built from atoms with fixed, usually repulsive interactions,' describes Dr Manz. 'This leads to fundamental phase diffusion, severely limiting the operation time of the interferometer.'

If this issue can't be solved, the entire approach would offer no improvement over previous devices, entirely defeating the point of using BECs in the first place. To overcome this next roadblock, Dr Manz and Dr Schumm aim to implement new techniques to control the interactions of individual atoms during the interferometer sequence. This will involve changing the composition of the BEC itself – from the rubidium atoms used in their previous experiments, with another, better-suited element.

Conceiving the iWave

Unlike the case for rubidium, interactions between atoms of caesium can be tuned using relatively weak magnetic fields. By trapping caesium BECs within optical double-well potentials, the researchers could ensure that the gases became trapped for seconds, avoiding the diffusion that had hindered their previous efforts. 'We will aim at the realisation of matter-wave optics using caesium atoms, where atom interactions can be dynamically adjusted,' Dr Manz continues. 'This should allow us to extend the interferometer operation time beyond what is accessible in other approaches and reach new regimes of sensitivity.'

The researchers would require a reliable new platform to implement this upgrade. They now intend for this to take the form of a highly compact, easily tuneable micro-fabricated chip – dubbed the 'iWave'. 'Our trusted workhorse for this endeavour is a so-called atomchip,' says Dr Schumm. 'Such chips provide tight magnetic trapping configurations and allow for near field manipulation with radiofrequency and microwave fields, and allow for close optical access for trapping and imaging with laser techniques.'

Although this setup has yet to be realised, Drs Manz and Schumm are already envisaging the new experiments that iWave will enable, through the ongoing control of caesium BECs during interferometry.

Measuring Gravity's Variation

One particular application the researchers envisage for iWave is a fundamental test of the Earth's gravitational field. Although we perceive the force of gravity as being uniform no matter where we stand on Earth's surface, this isn't strictly true. In reality, a wide variety of structures and mechanisms will vary the force in ways too subtle for our bodies to perceive, including mountains, ocean tides, and a slightly bulging equator. Drs Manz and Schumm hope that their device will one day allow researchers to probe these variations in unprecedented levels of detail, once it has been implemented onto their proposed 'tiltmeter'.

'The setup we propose is designed to measure feeble tilts of the direction of gravitational acceleration,' Dr Schumm explains. 'The plumb line of gravity exhibits interesting dynamics on daily timescales due to tides, celestial mechanics, processes of the Earth's interior and several others. We are working towards a local probe of gravitational gradients and forces, which implies keeping the setup as compact as possible, and at the same time being ridged enough to be tilted and rotated during a measurement campaign.'

Once completed, Drs Manz and Schumm predict that iWave will be so accurate that it will enable them to detect tidal deformations of the Earth's crust from the comfort of their lab in Vienna.

New Possibilities

The influence of quantum mechanics is now becoming spread across an increasingly diverse range of fields in physics. Now, thanks to the research of Dr Manz and Dr Schumm, this could soon extend to interferometry. If fully realised, the iWave will be able to pick up phase differences between split beams 10 times more precisely than conventional, light-based devices. The team will now continue working towards this goal in earnest, and could soon enable the most intricate ever analyses of the Earth's gravitational field to take place in the coming years.



Meet the researchers

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Dr Stephanie Manz achieved her PhD in Physics at Vienna University of Technology in 2010. She then went on to work as a postdoctoral fellow at institutions including the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, where she became a group leader in 2016. She returned to TU Vienna in 2017 as an assistant postdoc. Dr Manz's main research interests include quantum and matter wave optics, ultracold atom physics, electron diffraction, and the imaging of biological samples.

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Dr Thorsten Schumm completed his PhD in Physics at Paris-Sud University in 2006. He then worked as an Assistant Professor at Vienna University of Technology's Institute of Atomic and Subatomic Physics, before becoming the leader of the Quantum Metrology group in 2011. His broader research interests involve using the effects of quantum mechanics to construct high precision measurement devices and sensors. Through his research, Dr Schumm aims to realise devices including atomic clocks, matter-wave interferometers, and precision lasers.

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FUNDING

TU Wien (startup funding)
Austrian Science funds (FWF) Project P 31262
ÖAW discovery project microTASC

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NEW FRONTIERS OF SOUND: A QUIET REVOLUTION

Sound waves are all around us. They govern vibrations from the sweetest of sound to the most destructive earthquakes. Now, a team of researchers across the US has embarked on an ambitious project, named 'New Frontiers of Sound', which will pave the way for advanced technologies that operate using sound waves. Combining the expertise of more than 30 leading scientists and engineers from across the field of acoustics, the project promises to discover new properties of sound, while offering exciting opportunities for researchers from a diverse range of backgrounds.

Acoustic Waves

Although we spend little time thinking about them, sound waves constantly surround us, and permeate virtually every aspect of our lives. Scientifically, they are called 'acoustic' waves of compression and decompression, which propagate through materials as atoms and molecules bump into each other in chain reactions of energy exchange. These processes are now well understood by physicists, but, until now, they have not been widely exploited in the latest technologies.

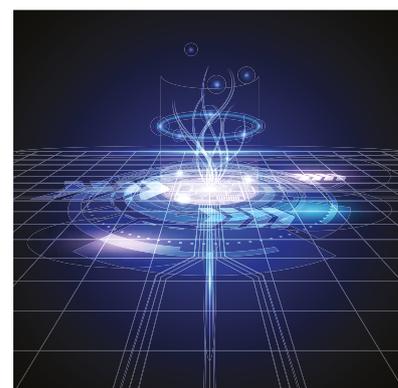
In recent years, the study and application of acoustic waves has been somewhat eclipsed by the field of optics, which exploits the properties of light waves. However, these two phenomena share many similarities, for instance, they obey analogous governing mathematical equations.

The New Frontiers of Sound (NewFoS) team believes that, since sound offers fundamentally different properties to light, this overshadowing has been preventing many exciting acoustics-based technologies from coming to

fruition. Through the NewFoS project, the researchers will focus on various areas and applications of sound wave manipulation, combining their expertise to rectify this issue. 'We will leverage the analogies between sound and light to bring powerful concepts demonstrated with light to totally unexplored venues to control sound propagation,' explains Dr Andrea Alù, one of the team leaders on the project.

Exceptional Points

Dr Alù and his colleagues at the City University of New York have explored the properties of 'singularities' in models of physical systems. At these so-called 'exceptional points', the mathematics needed to describe a system's response becomes entirely different from that used for conventional systems. So far, Dr Alù's work on exceptional points has been based on rare types of optical systems that exchange energy with their surrounding environments, making them useful for manipulating light waves in exotic ways.



These manipulations can be practically achieved using 'photonic' systems, which comprise engineered materials with features just a few nanometres across. Through experiments with these nanostructures, Dr Alù's team determined that these features are ideally suited for enhancing sensitivity and manipulating light in highly unusual ways. This discovery yielded important insights for optical applications, including ultrasensitive measurements and better control over lasers. Through NewFoS, these findings will be extended to acoustic waves – with important implications for a wide range of sound-based technologies.



Breaking Symmetry

Most systems that transport energy are symmetric, which means that the amount of energy transmitted from a source to a receiver remains unchanged when the two devices are switched around. This phenomenon is known as reciprocity. ‘Listening to an echo is experiencing reciprocity,’ says Dr Chiara Daraio, another team lead on the project. ‘Hearing attenuation of sound intensity in a forest due to scattering by trees is experiencing reciprocity, as scattering leads to energy loss.’

At the California Institute of Technology, Dr Daraio’s team studied systems in which symmetry can be broken through the principle of ‘nonreciprocity’, meaning that if the source and receiver are swapped, and the direction of energy flow is reversed, a different amount of energy is exchanged between them. ‘Nonreciprocity can be used to create sound-based low energy loss devices and make the battery of your mobile device last longer,’ explains Dr Daraio.

Dr Daraio’s group uses advanced calculations and experiments to produce a new material with a repeating yet asymmetrical structure. As they hoped, the researchers found that nonreciprocity could emerge in different systems and at different

frequencies, contributing to the design of one-way transport for acoustic waves – similar to that observed in electrical diodes. In addition, they identified the mechanisms responsible for this symmetry breaking – which would prove critical for the new devices and technologies planned as part of the NewFoS project.

One-way Travel

On larger scales than those investigated by Dr Daraio, symmetry breaking can occur in acoustic waves with a wide variety of shapes – which can be quantified by their wavelengths and amplitudes. NewFoS team lead Dr Massimo Ruzzene at the University of Colorado, Boulder investigated how the most extreme form of nonreciprocity can be recreated in acoustic waves: a completely one-way flow of sound, where no energy would be transmitted if a source and receiver were switched. To do this, his team devised a setup in which a beam of aluminium was partially covered in tightly packed, repeating arrays of patches that impart mechanical forces as they gather electrical charge. These patches were then connected to circuits and switches that periodically varied the mechanical properties of the beam over time as the waves passed through. Through experiments, Dr Ruzzene and his colleagues demonstrated that within a

certain band of frequencies, the beam could be manipulated to allow waves to freely travel in one direction, but completely block them in the other.

Quantum-like Sound Waves

At the same time as these studies, project lead Dr Pierre Deymier at the University of Arizona focused on the intriguing similarities between acoustic waves and ‘entangled’ quantum particles – one of the most famous and mysterious properties of quantum mechanics. The phenomenon describes how pairs of particles can stay linked to each other, even when they become separated by large distances. Importantly for Dr Deymier’s team, entanglement is also comparable to a property that emerges in propagating waves, known as ‘nonseparable’ states. In previous studies, nonseparable states have been observed experimentally using laser beams, but not with sound waves.

For the first time, Dr Deymier and his colleagues demonstrated this using a specialised ‘waveguide’ – an instrument typically used to direct waves along particular paths while sustaining minimal losses. In this case, nonseparable states were produced by stacking multiple sound waves on top of each other and linking them to the elastic waveguide through which they propagated. This setup allowed the researchers to carefully prepare and tune the shapes of the intricately connected waves as they travelled. At last, this result opened a clear door to the application of sound in modern technologies.

Sensing Forests

In addition to this study, Dr Deymier has explored how acoustic wave sensing could provide useful new ways to monitor the distribution of vegetation across the Earth’s surface. In this study, his team introduced a new technique for exploiting acoustic waves that travel through the ground, such as seismic waves emanating from earthquakes,



which become scattered and distorted by the roots of trees. Using simulated model forests, Dr Deymier's team calculated how these waves would respond to different arrangements and densities of trees.

The researchers found that acoustic waves in the ground are, in fact, extremely sensitive to these arrangements – displaying characteristic scattering patterns that depend strongly on tree distribution. They now hope that their results could lead to important new ways to characterise tree distributions, with applications including improvements to forest management and conservation, especially in more remote areas. Overall, the study clearly demonstrated just how broad the potential benefits of acoustic science can be.

New Frontiers of Sound

Each of these lead researchers, as well as the wider NewFoS team, foresees a 'quiet revolution' in the field of 'topological acoustics'. Now teaming up to bring sound to the forefront of scientific research, they are joined by an educational team led by Dr Sara Chavarria at the University of Arizona. Through this program, NewFoS will also promote greater involvement of researchers in typically underrepresented demographics.

The team has set out three goals for achieving these results. Firstly, the researchers will develop new techniques for producing miniaturised devices that can process large amounts of information encoded into sound waves. Secondly, they aim to produce acoustic wave-generating devices that offer far more tuneability than their previous counterparts. Finally, they will develop accurate acoustic sensors embedded into materials that could become invaluable for monitoring the infrastructures of technologically integrated 'smart cities' – all with lower signal losses than previous devices.

The NewFoS team hopes that by realising these aims, they will 'maximise the positive societal impacts from the pursuit of a new science of sound for information processing, communications, and sensing, and to leverage these societal impacts to foster successful and integrated transitions along education-to-professional career paths for a diverse workforce.'

Setting Out a Mission Plan

Ultimately, the NewFoS team hopes that their work will enable us to fully exploit the physical properties of sound waves for the broadest societal benefits, and attract the interest of partners in industry. At the same time, they will develop programs to educate and mentor a workforce encompassing researchers from a diverse variety of backgrounds and demographics. To do this, the NewFoS researchers have drawn out a mission plan centred around three central areas.

Firstly, the team will use advanced data science to build new materials and structures – combining their expertise to make informed decisions of how to manipulate sound waves in the most effective ways. Secondly, they will fabricate miniaturised devices that incorporate these materials using techniques such as 3D printing, which will enable intricate, repeating structures to be fabricated on small scales. Finally, they will develop techniques for incorporating sound waves from across the spectrum of acoustic frequencies, keeping their applications as broad as possible.

New Opportunities for Sound

As the modern technological landscape becomes ever more diverse and expansive, the NewFoS team hopes that their project will accelerate an expansion of the role that acoustic waves play in driving progress further. Their efforts will unite groups as wide-ranging as technologists, researchers, leaders, and policymakers to realise these goals, incorporating a combination of cutting-edge science and coordinated collaboration.

The researchers now hope that with the success of NewFoS, the science of sound may soon play a greater role in improving our everyday lives. 'We imagine a world in which miniaturised devices process massive sound-encoded information in way current computers cannot; acoustic wave devices enable a generation revolution in low loss, tunable, multifunctional wireless technologies; and embedded, distributed acoustic-sensors with high sensitivity and selectivity reveal and monitor the infrastructure integrity of smart cities and augment human performance in the work environment,' concludes Dr Deymier.

Meet the researchers



Dr Andrea Alù

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Dr Andrea Alù received his PhD from the University of Roma Tre, Italy, in 2007. He was

the Temple Foundation Endowed Professor at UT Austin until 2018, when he became the founding director of the Photonics Initiative at the Advanced Science Research Center at the City University of New York (CUNY) and Einstein Professor at the CUNY Graduate Center. Dr Alù's research focuses on a wide range of research interests, from nano-optics and photonics to acoustics and metamaterials.

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Dr Pierre Deymier completed his PhD at Massachusetts Institute of Technology in

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Alexander Khanikaev, CUNY

Derrick Hylton, Spelman College

FUNDING

National Science Foundation, Emerging Frontiers in Research and Innovation Program



PLASMA BUBBLES AFTER SUNSET: SIMULATING INSTABILITIES IN THE IONOSPHERE

Many kilometres above the Earth's equatorial region, something strange occurs for several hours in the late evening: vast bubbles of plasma form in the upper atmosphere, which quickly rise upwards into space. **Dr Joe Huba** at Syntek Technologies in Virginia aims to gain a better understanding of this complex process, by recreating it through computer simulations. His team's work is providing researchers with a more complete understanding of Earth's atmosphere, and could also provide critical insights for satellite systems that communicate using radio waves, as well as global positioning systems.



Earth's Ionosphere

If you look at a picture of Earth taken from space, the atmosphere will appear as a thin, fragile layer surrounding our home planet. Yet as we can clearly see by simply looking up at the sky, there is a diverse range of dynamic physical processes at play within the atmosphere, giving rise to effects including the weather we experience on Earth's surface.

At different altitudes, variations in air density, temperature and wind speed can have significant influences over these processes, resulting in several distinctive layers, each with its own

defining characteristics. Among these layers is a region named the 'ionosphere', which extends from 60 kilometres to over a thousand kilometres. This layer's defining characteristic is that the atoms and molecules it contains are partially ionised by powerful ultraviolet radiation from the sun.

The neutral atmosphere, known as the thermosphere at ionospheric altitudes, plays an important role in the dynamics of the ionosphere. Thermospheric winds interact with the plasma and generate large-scale electric fields, which can transport the plasma in altitude and latitude.

Within the ionosphere, several smaller regions can also be found. Among them is a high concentration of plasma named the F-region, situated between 150 and 800 kilometres above sea level. As many physicists are well aware, the intricately complex motions of plasma particles can give rise to many interesting behaviours, making the F-region an especially interesting part of the atmosphere. In the ionosphere above Earth's tropics, one particularly intriguing display begins to take place after sunset.

Instabilities in Immiscible Fluids

On smaller scales, the physics underlying this effect can be seen in the interaction between two immiscible fluids, such as oil and water. When the denser fluid is supported by the less dense fluid, an instability arises that creates a 'bubble' inside the denser fluid. This bubble accelerates and expands as it travels upwards into the denser fluid. This fluid instability is known as the Rayleigh-Taylor instability.



This complex scenario can be found in a wide range of situations in nature, from the clouds thrown up by volcanic eruptions, to cosmic explosions created by supernovae. To study them, researchers can construct computer simulations that recreate the properties of each fluid, enabling them to accurately reproduce the effects of instability.

In the lower latitudes surrounding Earth's equator, a comparable effect emerges in the ionosphere's F-region, which could be studied through similar simulations in principle. However, this situation is more complex than many cases studied previously – creating a unique set of challenges for Dr Joe Huba and his colleagues.

Equatorial Spread F

In the evening, after sunset, the ionosphere can be suddenly lifted to higher altitudes because of the electric field generated by the thermospheric wind. Under these circumstances, a sharp density gradient develops with the electron density increasing with altitude. The situation becomes similar to oil and water: a dense (heavy) plasma is supported by a less dense (light) plasma that becomes unstable. Irregularities can form large 'bubbles' of plasma, often tens of kilometres across.

These bubbles will then rise rapidly towards high altitudes, expanding and accelerating in the process. Afterwards, they can remain for several hours after sunset and sometimes past midnight. Now known as the 'equatorial spread F' (ESF), this phenomenon has a profound impact on the behaviour of the ionosphere surrounding the bubbles. In turn, it also has a significant effect on some of the radiation passing through the ionosphere – which cannot be ignored in the modern age of communication.

Unwanted Effects from Scintillation

For astronomers, an effect known as 'scintillation' is an ever-present challenge. Most commonly, it describes the random fluctuations experienced by radio waves as they pass through the streams of charged particles generated by the sun – known as the solar wind.

The effect is comparable to the twinkling we see when we look up at the stars at night. In this case, random turbulence in the atmosphere slightly diverts the paths of light emitted by stars, which we observe as twinkling. Similarly, radio waves can fluctuate as they pass through charged solar wind, causing inconvenient distortions of the signals emitted by distant astronomical objects due to effects including absorption, scattering, and frequency shifts.

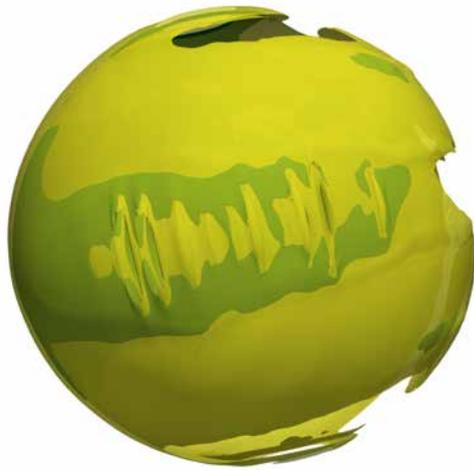
Dr Huba's team notes that the effect can become distinctly more noticeable for radio waves passing through the ionosphere at just the wrong time. As the plasma bubbles produced by ESF rise to high altitudes, they will create enormous disturbances in the rest of the ionosphere, causing the layer to become unstable to shorter wavelength irregularities (a few centimetres to hundreds of meters). When this happens, the resulting scintillation of radio signals can become so strong that it renders them unrecognisable by the time they reach Earth. Yet while the bubbles occur infrequently enough to not be a significant problem for radio astronomers, the case is different for systems that depend on highly accurate signal transmissions.

Disrupting Satellites

In order to operate effectively, many of the satellites we now rely upon in our everyday lives must continually hover over a single point on Earth's surface. To do this, they occupy a highly specific position in space called 'geostationary orbit' – consisting of a ring situated above the Earth's equator. Today, this ring is home to satellites used for applications including communication, navigation, and weather forecasting.

The positioning of geostationary orbit presents a problem: the radio waves that its satellites use to communicate with facilities on Earth must often pass through the equatorial F-region, where any scintillation can cause significant disruption to signal exchanges that require pinpoint precision.

As an example, global navigation systems are required to measure the exact times taken for radio waves to travel between different satellites in an array, and a single device on



Global electron density (green represents denser regions and yellow indicates lower density). The corrugated structure in the density is a result of plasma bubbles at lower altitudes rising to higher altitudes.

Earth. If any of these signals pass through a plasma bubble, this timing information could be completely disrupted, leading to potentially damaging inaccuracies in global positioning. Without any way to prepare for these fluctuations, the systems that many people depend upon can become far less reliable for several critical hours in the late evening.

Barriers to Accurate Models

To alleviate these problems, physicists need to build computer simulations that can model, and subsequently forecast, when ESF bubbles will occur – affording the operators of satellite systems critical time to prepare for them. Yet as is the case for many simulations involving plasma, these models are notoriously challenging to build, since they must account for the intricate webs of interactions between the charged particles they contain. For a situation as complex as ESF, bubble plasma evolution is particularly difficult to predict.

In the past, researchers have simplified the situation by only simulating a more easily manageable 2D ionosphere. Later advances in computing technology have more recently allowed

for 3D simulations. However, all of these efforts have so far faced several shortcomings: they model a limited region of the ionosphere, usually a few degrees in longitude and tens of degrees in latitude, and neglect realistic thermospheric waves.

Simulating Plasma Bubbles

Through their research, Dr Huba and his colleagues have accounted for this behaviour for the first time, by combining two global, first-principles atmospheric models: the whole atmosphere model WACCM-X and the ionosphere model SAMI3. Moreover, these models use very high grid resolutions, on the order of 70 kilometres. This allowed the team to recreate entire equatorial ionosphere driven by a realistic thermosphere model that includes atmospheric waves, such as gravity waves which can act as ‘seeds’ to trigger the instability.

To test the performance of their approach, they carried out the two simulation studies at two different times of year under different geophysical conditions: the ‘March case’ for low solar activity and the ‘July case’ for high solar activity.

Without any further input, Dr Huba and his colleagues found that their simulation self-consistently generated rising plasma bubbles. Furthermore, they found that in the March case – when the sun’s activity was lower – the bubbles penetrated to the upper reaches of the F-region, around 800 kilometres above sea level, where they persisted until after midnight. In contrast, this didn’t happen in the July simulation, during higher solar activity. Understanding why bubbles occur on some nights but not others is one of mysteries that these simulations hope to unravel.

The team compared the results to observations made by NASA’s GOLD mission, which continually monitors the ionosphere. Unexpectedly, the simulated behaviour was highly consistent with GOLD’s observations, proving that their approach resulted in the first reliable simulations of ESF plasma bubbles.

Informing Future Improvements

The reliability of the team’s simulation represents a significant step forward in our ability to understand the physics underlying ESF, and to prepare for the inconveniences created by rising plasma bubbles.

As we come to increasingly rely on satellites for communication and navigation, the outcomes of their research could soon lead to important new measures to safeguard and improve these systems. Through future research, they could also yield intriguing insights into the complex processes that play out above our heads, helping researchers in many different fields to understand more about the Earth’s atmosphere as a whole.



Meet the researcher

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Dr Joe Huba completed his PhD in theoretical plasma physics at the University of Maryland in 1975. Following his graduation, he joined the Naval Research Laboratory as an NRC post-doc and eventually became a staff member. Between 1995 and 2018, he headed the Space Plasma Physics Section, part of the Beam Physics Branch at the Naval Research Laboratory. He now works as a Senior Research Scientist at Syntek Technologies, whose clients include the US Federal government. Dr Huba's main research interests include boundaries and wave phenomena in plasma, processes involving Earth's upper atmosphere and magnetic field, and approaches to modelling these systems. Over decades of research, he has been dedicated to writing advanced computer code to simulate these systems, which incorporate algorithms capable of simulating their sheer complexity.

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The original ionosphere model, SAMI3, was developed by Drs Huba and Joyce. Dr Joyce played a critical role in the code's development but sadly passed away in 2011.

FUNDING

National Science Foundation (NSF)
National Aeronautics and Space Administration (NASA)

FURTHER READING

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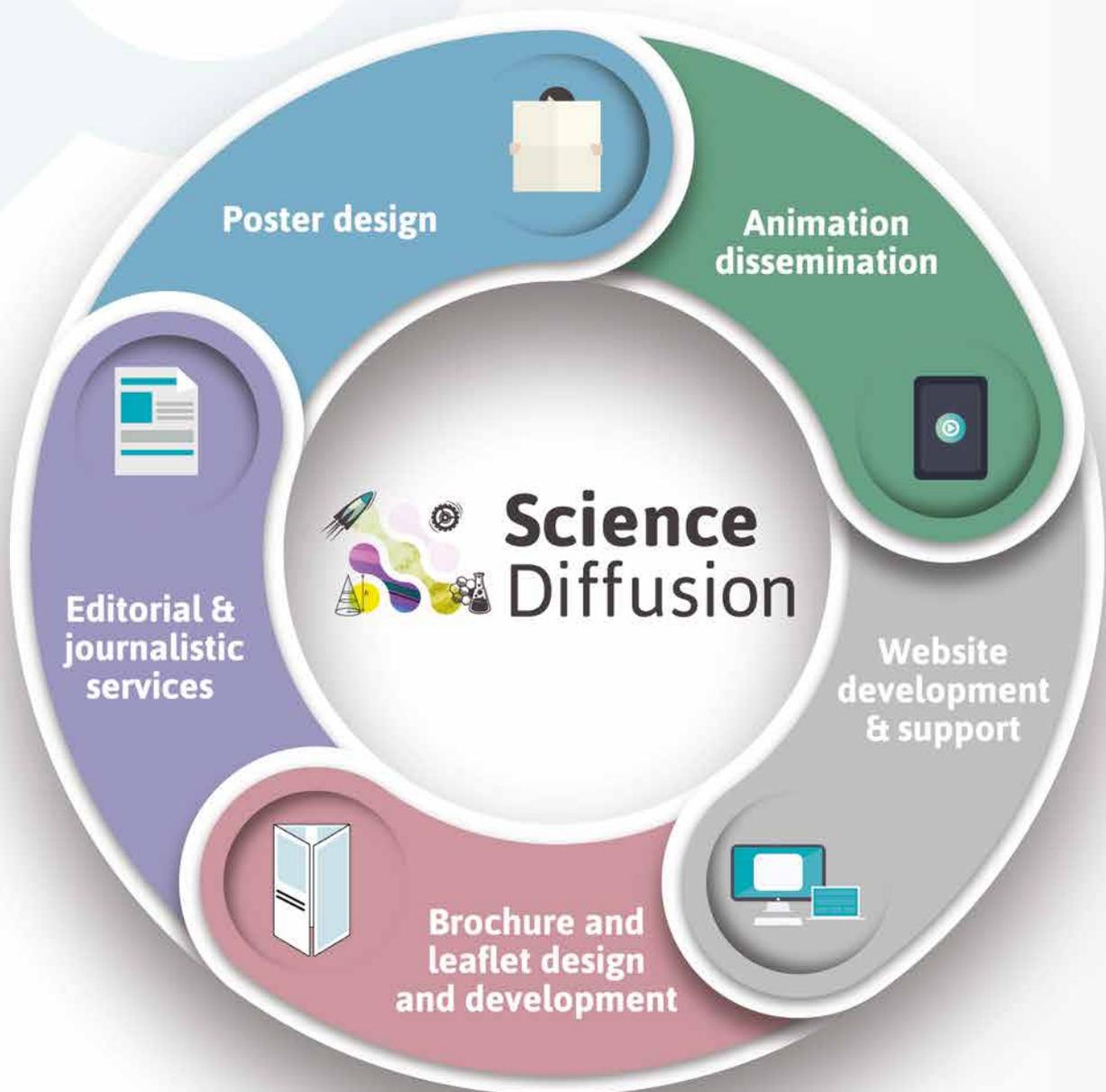
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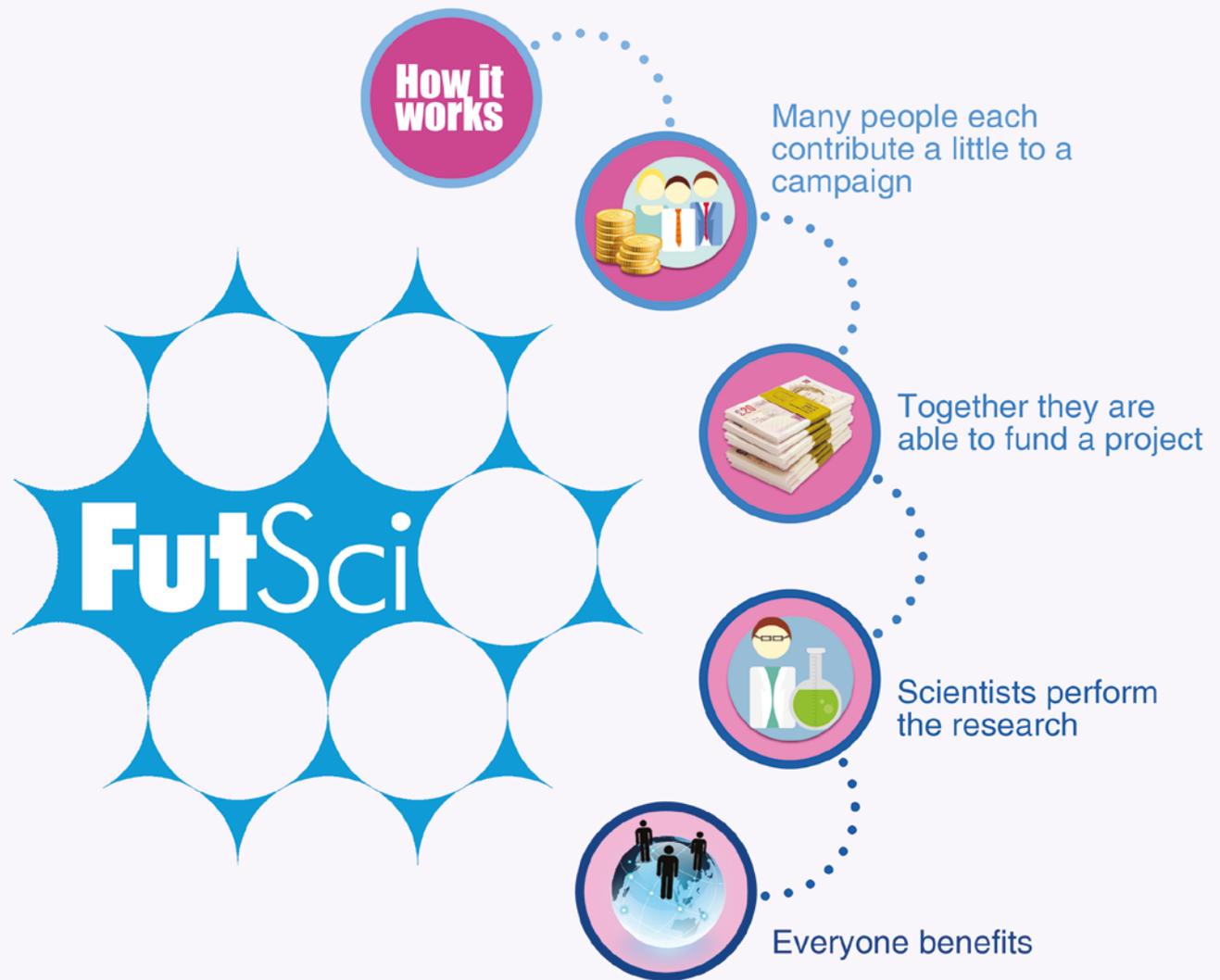
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