Scientia

SHIFTING PARADIGMS IN PHYSICS AND ENGINEERING

HIGHLIGHTS:

- The Unexpected Spirals of Electron Density
- Catching the Wind: Understanding the Dynamics of Renewable Energy
- Hope for Humanity in the Energy Crisis: Astronomical Jets in a Lab
- Mixing Analogue and Digital Computers: The Future is Hybrid

EXCLUSIVE:

- CERN – The European Organisation for Nuclear Research

Issue: #115

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WELCOME...

In this electrifying edition of Scientia, we showcase the work of various research groups across the globe, each dedicated to shifting paradigms in the diverse fields of physical science and engineering.

To begin, we delve deep into the most fundamental building blocks of our Universe – the elementary particles. Here, we explore everything from the trillions of cosmic neutrinos that pass through our bodies every second, to the antimatter positrons used in medical imaging technology. We also feature an exclusive interview with Professor Tara Shears about her team's recent discovery of five particles at CERN. We then jump up the scales – first showcasing the latest paradigm shifts in molecular science, followed by recent breakthroughs in nanotechnology. Finally, we introduce a team of scientists who investigate (amongst other things) the dynamic behaviour of raindrops, which may help us to more accurately forecast extreme weather events caused by climate change.

In our middle section of the edition, we meet many remarkable researchers – each dedicated to combatting climate change and solving the energy crisis through developing and improving sustainable energy technologies. Here, we feature several varied and promising research projects, from boosting the efficiency of wind turbines, to creating the most energy-dense lithium-ion battery, and finally, to realising controlled nuclear fusion as a future power source.

Finally, we showcase the latest innovations in computer science and engineering, where we meet an incredible bunch of researchers, each aiming to improve our lives through enhancing our computing technologies. One team of researchers is combining analogue and digital computing to create a device capable of solving large sets of differential equations, while another has created an accurate and affordable virtual reality controller, which holds promise for numerous fields, including medicine, architecture and gaming.

From illuminating our understanding of the Universe, to combatting climate change and developing futuristic computing technologies, the research teams featured in this edition are certainly paving the way to a bright future for all.

Science Diffusion

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Published in the UK, by
Science Diffusion ltd

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

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Meet The Team...

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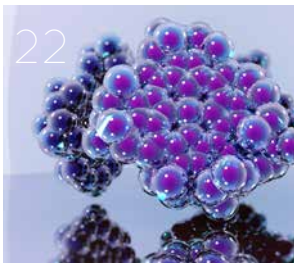
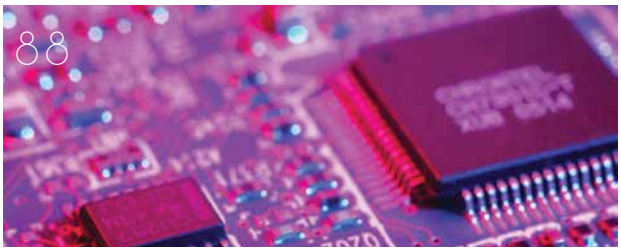
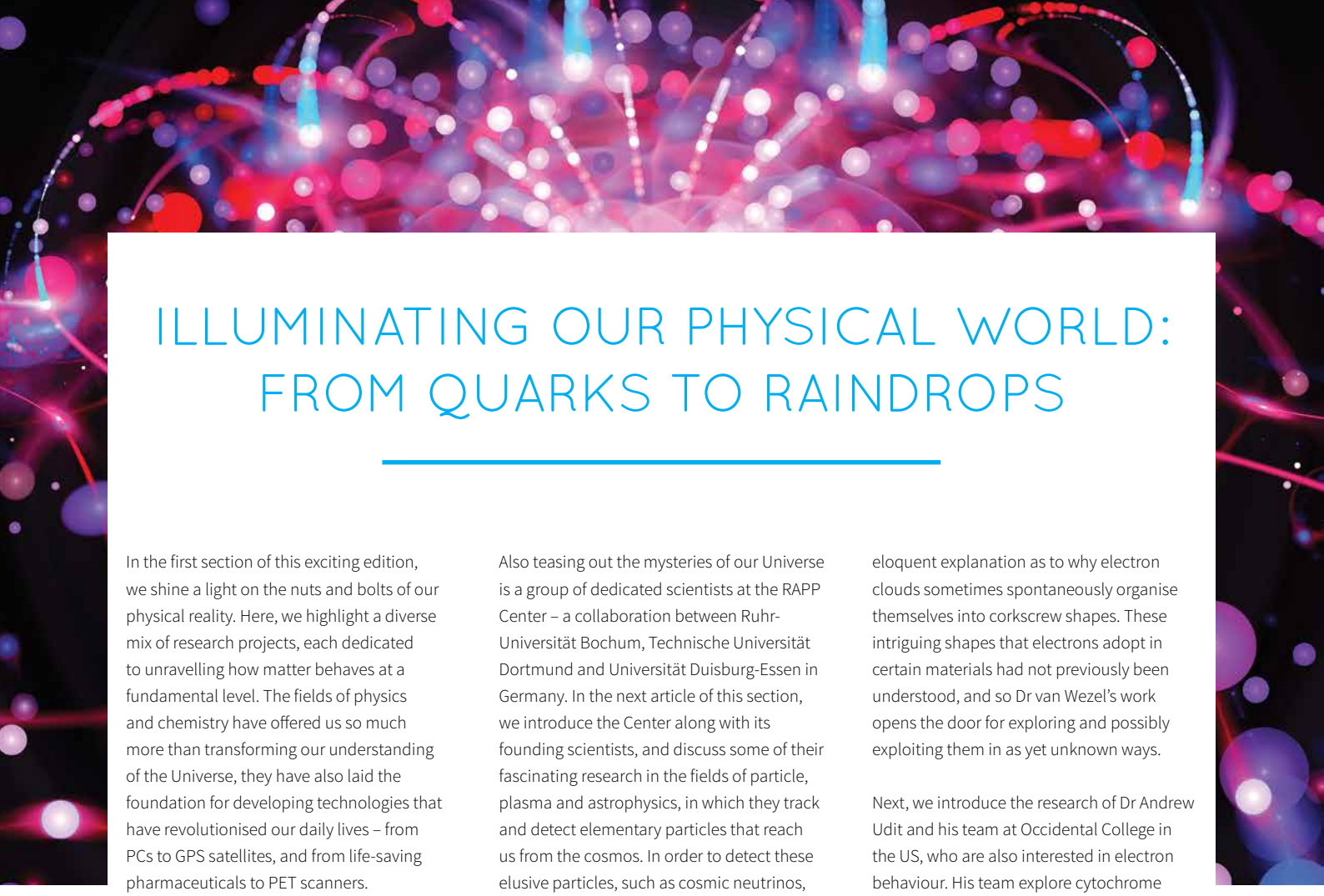






ILLUMINATING OUR PHYSICAL WORLD: FROM QUARKS TO RAINDROPS

In the first section of this exciting edition, we shine a light on the nuts and bolts of our physical reality. Here, we highlight a diverse mix of research projects, each dedicated to unravelling how matter behaves at a fundamental level. The fields of physics and chemistry have offered us so much more than transforming our understanding of the Universe, they have also laid the foundation for developing technologies that have revolutionised our daily lives – from PCs to GPS satellites, and from life-saving pharmaceuticals to PET scanners.

We start off by exploring the smallest units of matter – quarks, neutrinos, electrons, and even antimatter positrons – before leaping up the scales, first to molecules, then nanoparticles and finally, raindrops!

To open this section, we showcase a recent discovery made by scientists at CERN in Switzerland, of five previously-unseen subatomic particles. By forcing beams of high-speed protons to collide, the Large Hadron Collider (LHC) at CERN can cause this ordinary matter to break down, while the phenomenal energy available allows it to reappear in exotic forms. Under these extreme conditions, unusual particles that pop into existence offer us a brief glimpse into how matter might have behaved shortly after the Big Bang. On the 16th of March this year (2017), the LHCb team announced the discovery of five previously unknown particles, all found in a single analysis. These particles have been named the 'omega_c baryons', each composed of one 'charm' and two 'strange' quarks – exotic heavy analogues of the 'up' and 'down' quarks that make up the protons and neutrons of normal matter. In our exclusive interview, we have had the pleasure of speaking with Dr Tara Shears – one of the scientists behind this remarkable discovery.

Also teasing out the mysteries of our Universe is a group of dedicated scientists at the RAPP Center – a collaboration between Ruhr-Universität Bochum, Technische Universität Dortmund and Universität Duisburg-Essen in Germany. In the next article of this section, we introduce the Center along with its founding scientists, and discuss some of their fascinating research in the fields of particle, plasma and astrophysics, in which they track and detect elementary particles that reach us from the cosmos. In order to detect these elusive particles, such as cosmic neutrinos, RAPP Center researchers exploit the most sensitive state-of-the-art detector facilities, by collaborating with different facilities across the globe.

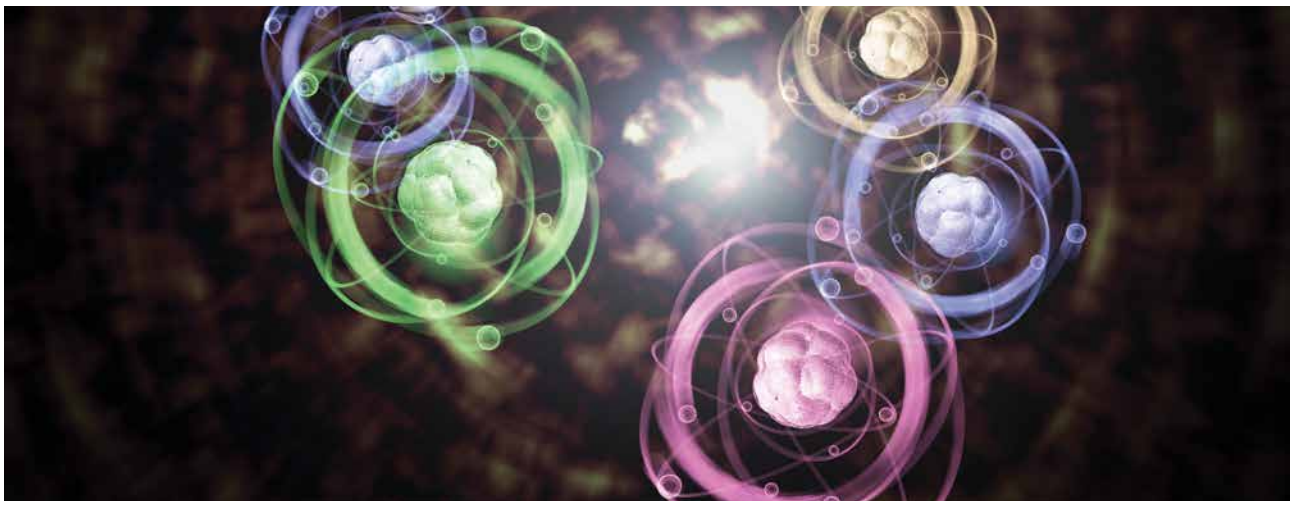
Next, we meet Dr Paul Lecoq and his team at CERN, who are taking advantage of the latest technologies in particle detection to design the world's most sensitive positron emission tomography (PET) scanner. As its name suggests, positron emission tomography is a diagnostic technique that relies on the use of positrons – the antimatter equivalent of electrons – to observe metabolic processes in the body. Here, we discuss the ground-breaking modifications that Dr Lecoq's team is making to current PET scanners, which will help physicians make more precise diagnoses, implement more accurate treatment plans and increase patient survival rates for a variety of conditions.

Our next article focuses on some of the intriguing behaviours of electrons. Electrons are themselves elementary particles, as they have no known substructure, just like their antimatter equivalent – the positron – discussed above, as well as quarks and neutrinos. Here, we showcase the work of Dr Jasper van Wezel and his team at the University of Amsterdam in the Netherlands, who have developed an eloquent explanation as to why electron clouds sometimes spontaneously organise themselves into corkscrew shapes. These intriguing shapes that electrons adopt in certain materials had not previously been understood, and so Dr van Wezel's work opens the door for exploring and possibly exploiting them in as yet unknown ways.

Next, we introduce the research of Dr Andrew Udit and his team at Occidental College in the US, who are also interested in electron behaviour. His team explore cytochrome P450 enzymes, which rely on electron transfer to power many different chemical reactions. Members of this large family of enzymes are found in every kingdom of life, where they play a huge number of different biological roles. Because of their diverse functions in the body, the potential uses for P450 enzymes are immense – so Dr Udit's team is working on developing a system that allows cytochrome P450 enzymes to be efficiently exploited for medical and industrial use.

Another scientist at the forefront of molecular science is Dr Bretislav Friedrich at the Fritz Haber Institute in Germany, who has devised new ways to align molecules in specific orientations, with the help of electromagnetic fields. In this next article of the magazine, we also discuss his team's mathematical quest to find exact solutions to the Schrödinger equation (the most ubiquitous equation in the field of quantum mechanics) to describe the interactions between molecules and the fields that coerce them into alignment.

Also working to control molecular behaviour are Dr Lisa Burden, Dr Daniel Burden and their colleagues at Wheaton College in the US. Similar to Dr Udit and his colleagues, this research team has taken inspiration from biology – this time to design nanometre-sized



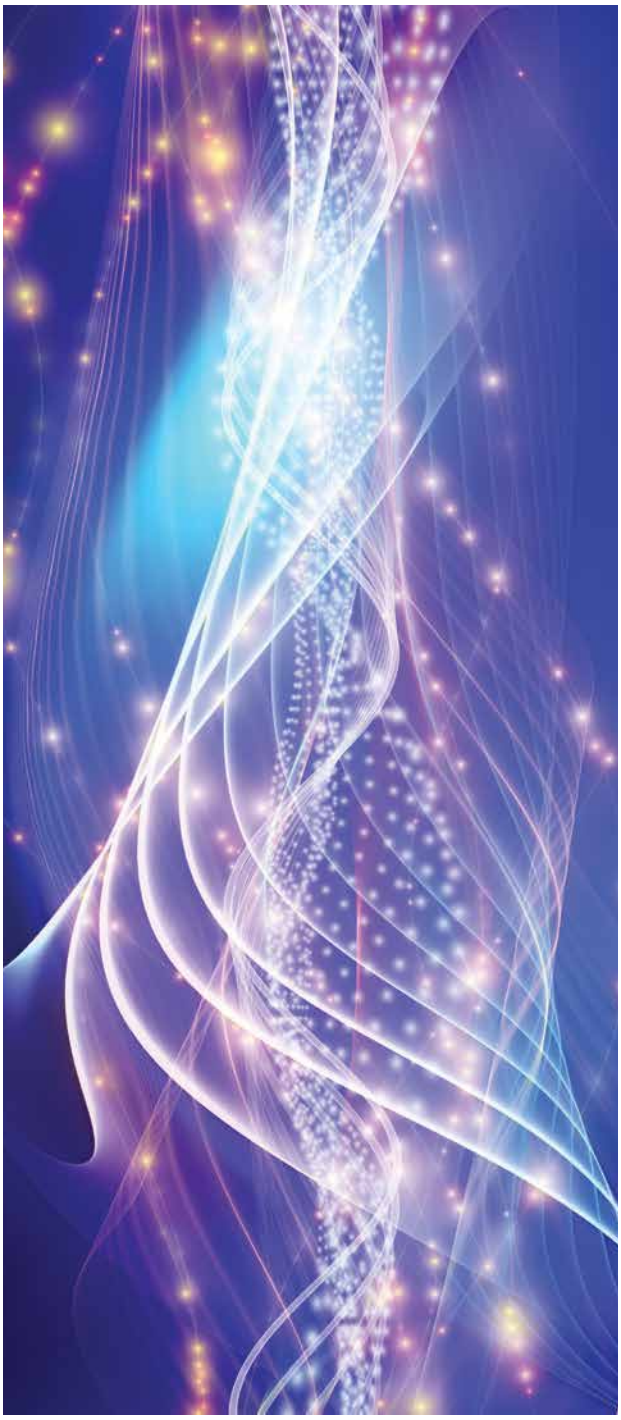
pores or valves embedded into a lipid layer that closely resembles a cell membrane. The team is working to find ways of precisely controlling the movement of molecules as they are transported in and out of these 'nanopores', which could allow the team to develop accurate chemical sensors. If realised, these membrane-based sensors and other similar devices could find numerous applications in many different fields, such as environmental monitoring, medical diagnostics and nanomedicine.

Indeed, the field of nanomedicine is experiencing rapid growth at present. However, since this discipline is still in its infancy, the long-term adverse effects of nanomaterials on the body are still poorly understood. To address this shortfall, the SmartNanoTox team was established, whose research we will introduce next in this section. Comprising experts in in-vivo toxicity from across Europe, the team is working to resolve the intricate mechanisms that underlie nanotoxicity, and to provide an efficient approach for predicting the toxicity of many different nanomaterials.

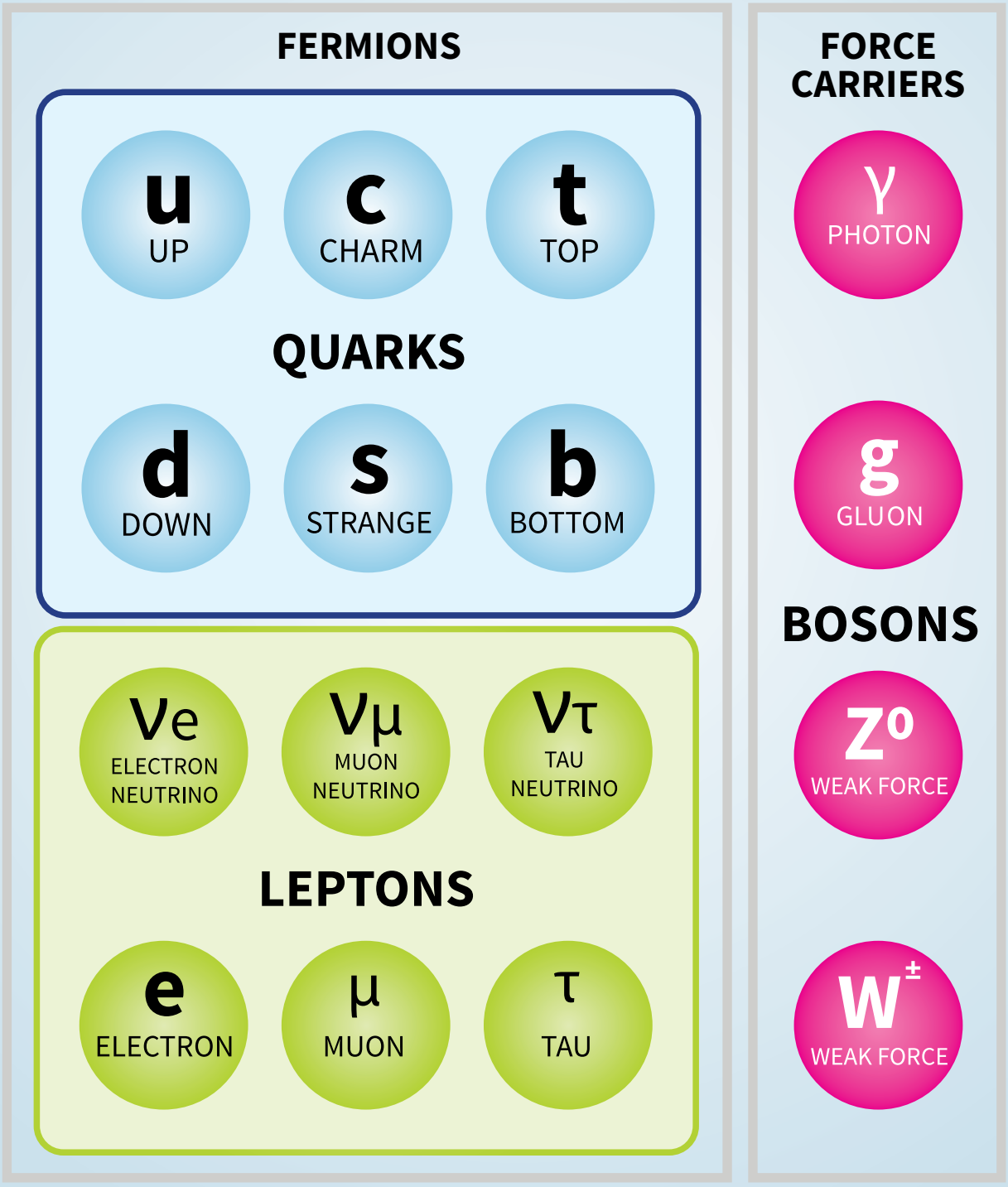
Next, we showcase the work of Dr Ning Pan at University of California, Davis, in the US, who has also been finding ways to accurately assess and predict the properties of materials. His team's work, however, concerns the properties of textile materials – such as the mechanical strength of rope and even the sensory properties of fabric. In one fascinating research direction, his team developed a mathematical model to predict the level of stress and friction experienced by a person wearing a garment with sleeves.

From here, we jump into the bewildering world of fluid dynamics, where we showcase two research projects dedicated to enhancing our understanding of this area. First, we highlight the work of Richard Miles at Texas A&M University, whose latest breakthrough involves a new technique to measure the velocities of high-speed fluids. His team's revolutionary approach – called FLEET – uses a laser and a camera to directly and non-intrusively measure the speeds of fluid flows and has the potential to make waves within many different industries.

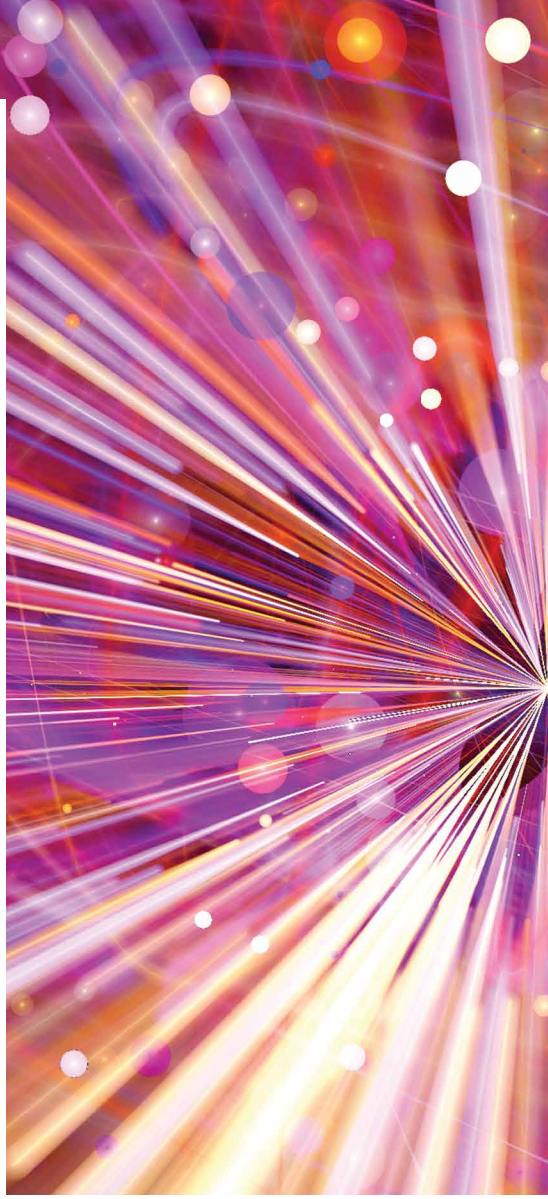
Our second project in the field of fluid dynamics is headed by Dr Lian-Ping Wang at the University of Delaware in the US. In this final article of the section, we showcase his team's work into understanding interactions between particles and fluid in turbulent flows. Their innovative models have greatly improved our ability to understand and predict many different phenomena, from localised rainfall patterns all the way through to particle transport in industrial processes.



ELEMENTARY PARTICLES IN THE STANDARD MODEL



FIVE NEW PARTICLES DISCOVERED AT CERN



CERN's Large Hadron Collider (LHC) is the largest and most powerful particle accelerator ever constructed. Featuring a 27-kilometre ring containing superconducting magnets, the LHC can accelerate protons to almost the speed of light, forcing proton beams travelling in opposite directions to collide. The enormous energy released in these high-speed collisions recreates, for a very short time, the inconceivably hot conditions of the early universe. Under these conditions, heavy quarks can pop into existence, giving rise to unusual particles that can be picked up by the LHC's detectors as they rapidly decay into normal matter. As one of the LHC's seven detector experiments, the LHCb experiment explores what happened directly after the Big Bang that allowed matter to survive and build the Universe. On the 16th of March this year, the LHCb team announced the discovery of five previously unknown particles, all found in a single analysis. Each particle is a different type of omega_c baryon, composed of one 'charm' and two 'strange' quarks – heavy analogues of the 'up' and 'down' quarks that make up the protons and neutrons of normal matter. In this exclusive interview, we have had the pleasure of speaking with Professor Tara Shears, one of the scientists behind this unusually fruitful discovery.

Please start by telling us a bit about these five new particles and their characteristics.

These new particles are exotic types of particles called baryons, which is an object made of three quarks. Quarks are the building blocks of matter and come in six different varieties. Collections of the most ubiquitous 'up' and 'down' type quarks form neutrons and protons, the baryons contained in atomic nuclei. But the other, rarer quarks can form baryons too. Our discovery concerns baryons made of one 'charm' and two 'strange' quarks, known as 'omega_c' baryons. The first omega_c baryon was discovered a few years ago, but that left many more excited (more massive) partners to find. LHCb has discovered five distinct excited state partners, dramatically extending our knowledge of this particular type of particle.

The new omega_c baryons are all formed of one charm and two strange quarks. What makes the particles different to each other is the configuration the quarks adopt inside them, giving different, characteristic values of quantities like angular momentum and spin to each new baryon. Each of the new baryon states also has a distinct value of mass, so unimaginatively we've included this in the name of each of them: the omega_c(3000), omega_c(3050), omega_c(3066), omega_c(3090) and omega_c(3119), where the number in the bracket is the baryon mass in particle physics units of MeV/c2 (a proton has a mass of 938 MeV/c2, for comparison).

Omega_c baryons exist for only a fraction of a second before decaying to other particles, so are quite hard to find. However, if you know the particles that omega_c baryons decay to and you can find them in your data, the task isn't impossible.

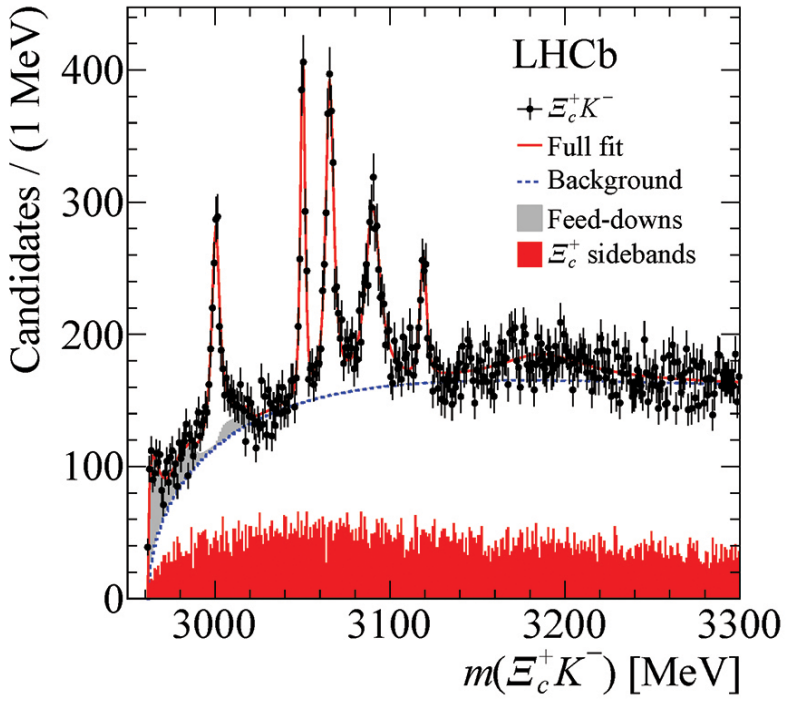
Do these specific particles exist in nature, or only under the extreme-energy conditions of the LHC? Had they been previously predicted by theory?

We expected these extra omega_c baryons to be out there. They are predicted to exist by our Standard Model particle physics theory, but that doesn't mean that predicting exactly where they exist is easy! So finding them is going to help us understand more about the forces that binds quarks together in baryons, and that is really valuable.

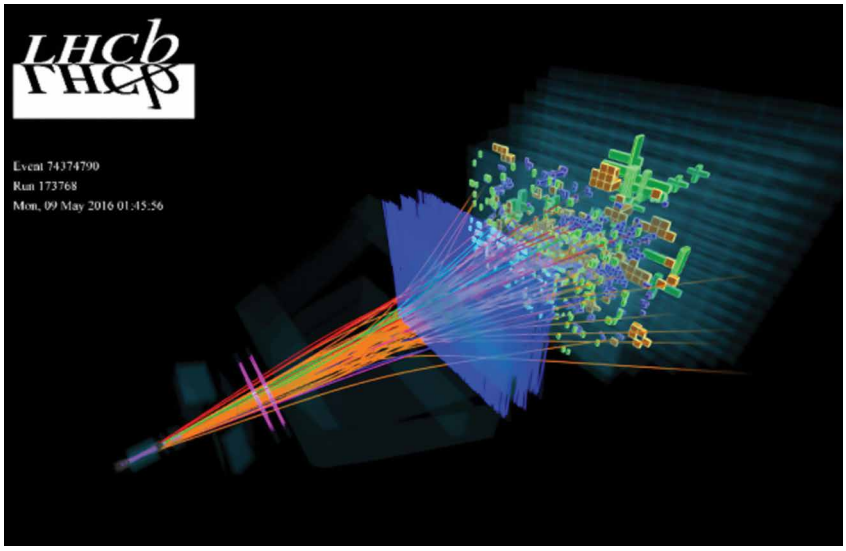
Having said that, you need a lot of energy to create an omega_c baryon, and they decay very quickly. So they only exist momentarily in high energy environments – whether those are LHC collisions, the high temperatures of the very early universe, or in high energy collisions of a cosmic ray with the Earth's atmosphere or surface.

All five particles were discovered in a single analysis – how rare is it to find so many unknown particles all at once? Were you and the rest of the LHCb team surprised at this?

I hesitate to say that waiting to find a new particle is a little like waiting for a bus without a timetable, and not knowing when it will turn up, but in this case the temptation is too great to resist. It's very rare to see so many new particles at the same time. Usually you concentrate on looking for one. It's just



Masses of candidate baryons passing the data selection. The red line shows the result of the fit, with 5 new particles revealing themselves as peaks, and the blue line shows the estimated background. CREDIT: LHCb collaboration



A typical LHCb event fully reconstructed. Particles identified as pions, kaon, etc. are shown in different colours. CREDIT: LHCb collaboration

that here the new particles had such similar properties, but were distinguishable, that they could all be found within the same data analysis and it was a case of find one, get four free.

Tell us a bit about the specialised capabilities of the LHCb detector, and how it detects particles of this kind.

LHCb is a superb piece of equipment and ideally suited to teasing out the traces of these new particles. For a start, it operates at the Large Hadron Collider and has access to the enormous datasets necessary to skim through to find traces of rare particles like these. Its particle detectors are designed to identify the experimental signature of short-lived particles, such as the omega_c baryon, in real time, allowing promising candidates to be selected and recorded. Other particle detectors identify the types of particles that

‘You need a lot of energy to create an omega_c baryon, and they decay very quickly’

the omega_c baryon decays to, allowing the full decay to be reconstructed and the omega_c itself to be identified. What’s unique about LHCb is that it has a unique, lower luminosity data taking mode at the LHC, and that allows us to study omega_c baryons with low backgrounds and high efficiency.

Explain what this new finding means for particle physics and quantum theory. Do you have any plans to probe these particles further?

We know that the strong force binds quarks together in baryons, and a description of how this works is contained in our Standard Model theory. However, the theory that describes the strong force is complicated and predicting exactly how quarks bind together is hard. These new measurements will help to refine that understanding. They will allow us not just to understand how quarks are bound in baryons, but potentially in more exotic types of particles containing four or five quarks too, particles that we are just starting to uncover in our data now.

Having seen these particles, now we want to know what they do, so I’m sure that a programme of omega_c baryon investigations will start. And our quest to understand the workings of the strong force will continue too, by probing the behaviour of quarks and the objects they form the constituents of, as precisely as we can.

https://lhcb.web.cern.ch/lhcb/

THE RAPP CENTER: SEARCHING FOR ANSWERS IN PLASMA-ASTROPARTICLE PHYSICS

The Ruhr Astroparticle and Plasma Physics (RAPP) Center was established in 2015 by Professor Julia Tjus and her colleagues within the University Alliance Ruhr – a collaboration between the three universities of the Ruhr area: Ruhr-Universität Bochum, Technische Universität Dortmund and Universität Duisburg-Essen. The Center is unique in the German research landscape, as it systematically combines theory and observations in particle, plasma and astrophysics in order to explore and understand the mysteries of the cosmos by tracking and detecting low- and high-energy elementary particles.

Astroparticle physics strives to explore and understand the extremely energetic particles that reach us from the depths of the cosmos. Because these particles are often charged, their paths are highly distorted by the magnetic fields that exist on large scales in and between galaxies in the Universe, making it difficult to trace high-energy cosmic rays to their sources. The description of cosmic ray signatures requires the combination of astrophysics, particle physics and plasma physics. The latter is used to properly describe the interaction of charged cosmic rays with magnetic fields, while particle physics is needed to understand cosmic ray interactions and signatures of dark matter. In fact, the theory and experiments adopted by astroparticle physicists use information from the entire electromagnetic spectrum in order to understand how cosmic rays travel through and influence the interstellar and intergalactic media, and also how particle interactions work at the highest energies.

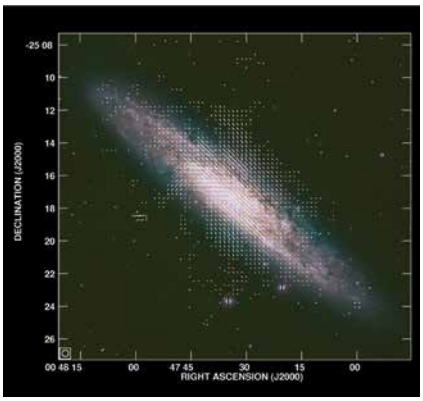
The interpretation of these multimessenger data requires a proper treatment of the basic physics involved. The intersection of particle, astro- and plasma physics can enable researchers to explore the different states of matter, with each discipline offering information on different physics regimes. Combining these pieces of information will lead to a more comprehensive view of the Universe. The RAPP Center is the first of its kind in Germany to systematically combine these methods. In doing so, scientists in the RAPP Center seek to contribute significantly to answering four of the central physics questions of this century, interconnected through the interaction and transport of cosmic rays:

- What is the origin of cosmic rays?
- What is the nature of neutrinos and dark matter?
- How does the interaction of cosmic rays influence the interstellar medium – from molecular clouds to protoplanetary disks?
- How are magnetic fields generated and maintained in the Universe?

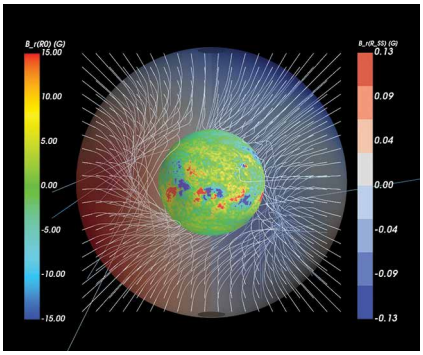
These questions share a common basis in that they take advantage of knowledge from the three subdisciplines of physics – plasma, astro- and particle physics – to find answers on a fundamental physics level.

A Center for Astro-, Particle and Plasma Physicists

In 2007, three German universities – Ruhr-Universität Bochum, Technische Universität Dortmund and Universität Duisburg-Essen – formed the University Alliance Ruhr (UAR). In 2010, the Alliance became home to the Mercator Research Center Ruhr (MERCUR) – a joint initiative for funding research projects. This created the basis for the emergence of the Ruhr Astroparticle and Plasma Physics Center (RAPP), which was established to provide a strong foundation for research efforts in plasma, astro- and particle physics in the Ruhr area. The close proximity of the three founding universities (within a range of only 20 kilometers) allows researchers to work together closely and collaborate on research and funding projects. In this context, the

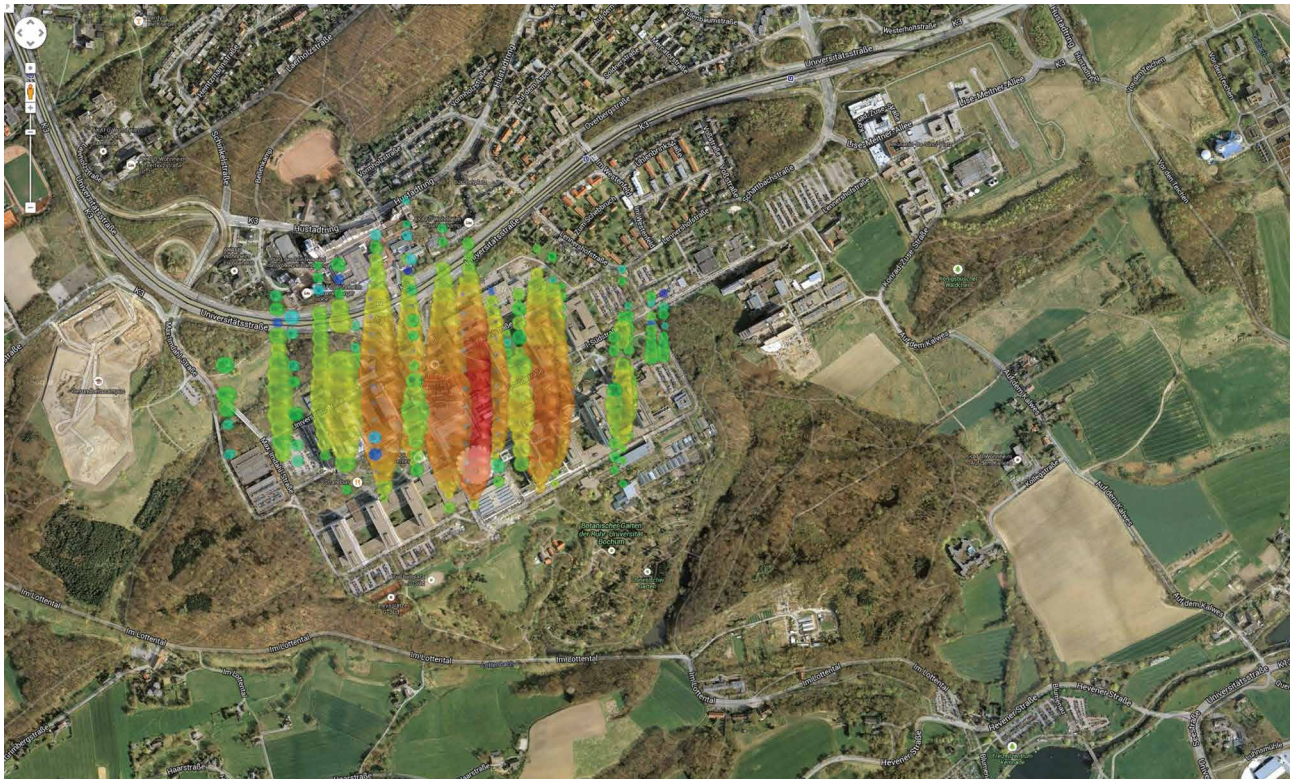


Multiwavelength view and the magnetic field structure of the galaxy NGC253 (provided by V. Heesen)



Cosmic ray transport in the solar magnetic field (published in: M. Kroll, PhD thesis, Ruhr-Universität Bochum, 06/2017)

‘Just imagine, we try to describe particle interactions at the sub-nanometer scale, after they have propagated over millions of light years.’



Bert over Bochum: a representation of the neutrino event named “Bert” detected by IceCube, shown projected to scale onto the Ruhr-Universität Bochum campus (map from Google Maps)

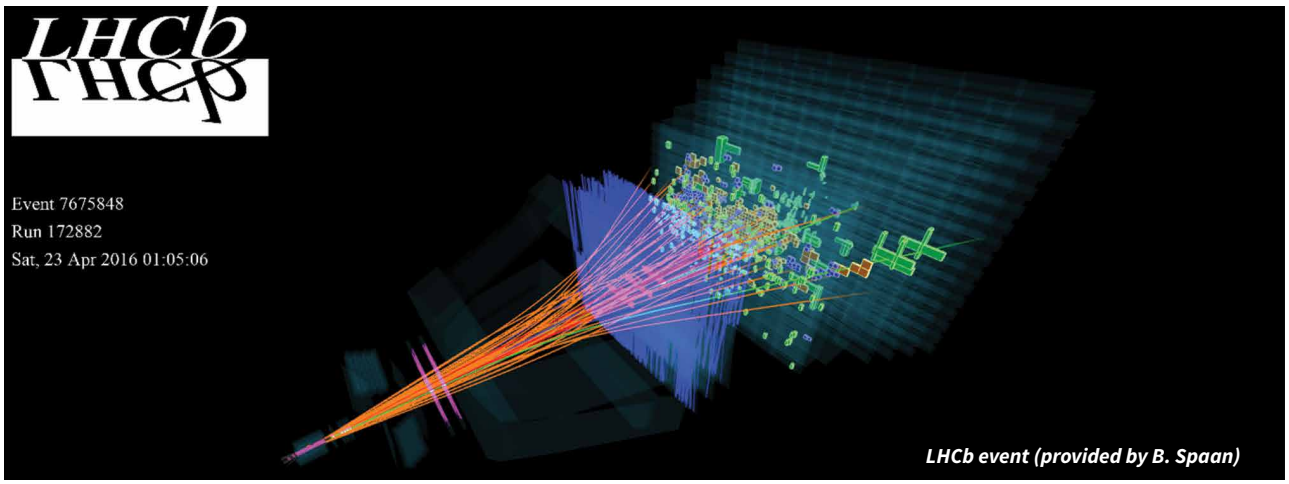
RAPP Center naturally came into existence as the brainchild of six professors from the University Alliance Ruhr – Professors Dettmar, Rhode, Schlickeiser, Spaan, Tjus and Wurm – who today are six of the 23 principal investigators of the Center.

The principle investigators are involved in a large number of large-scale experiments, among them the Large Hadron Collider at CERN, located in Geneva, Switzerland, and the planned Square Kilometer Array, set to become the world’s largest telescope array for the detection of radio waves, to be built in South Africa and Australia. A further example is the IceCube Neutrino Observatory located at the South Pole. IceCube is the world’s largest neutrino detector and comprises one cubic kilometer of instrumented ice, which makes for a rather literal name. Neutrinos, produced in the Earth’s atmosphere or originating from the cosmos, pass through IceCube and sometimes (but rather rarely) interact with the ice. Thus, the sheer volume of one cubic kilometer makes it just large enough to detect the very small signals from cosmic neutrinos. Given that neutrinos are extremely difficult to detect, the size of the instrumented volume increases the probability that some neutrinos will interact with it before exiting at the other side. Professors Rhode and Tjus have been working on IceCube (and its smaller predecessor AMANDA) since 1998 and 2003, respectively, contributing to the development of different analysis techniques like unfolding and stacking by adding information from the theoretical modelling of neutrino sources.

Cosmic Interactions: From Source to Signal

There is a strong connection between the fields of plasma and astrophysics, as the creation of magnetic fields in the Universe relies on the dynamics of plasma in the Universe – defined as a quasi-neutral gas composed of approximately the same number of particles with positive and negative charge. It is believed that the dynamics of this particle ensemble, possibly through interactions between the general background plasma and high-energy cosmic rays, is responsible for creating large- and small-scale magnetic fields in the Universe. Therefore, only the combination of plasma and astrophysics will be able to answer this fundamental question. Astroparticle physics was developed from particle physics, in that it studies elementary particles coming from astronomical sources. This field is also closely related to astrophysics, because it studies these particles in the context of cosmology.

At the same time, high-energy cosmic rays exceed energies that terrestrial particle accelerators can achieve – the highest energy detected for a cosmic particle can be compared with the energy of a tennis ball served at 200 kilometers per hour. The field of astroparticle physics seeks to understand how these particles can be accelerated to such extreme energies and what sources in the Universe are responsible. As acceleration processes are expected to arise due to non-uniformities in magnetic fields, plasma physics also plays an important role here. These highest-energy particles can reveal properties of elementary particles at an energy scale that cannot be probed using



LHCb event (provided by B. Spaan)

LOFAR station in Jülich (photo by E. Jütte)

man-made accelerators. The interplay between astro- and particle physics is therefore crucial to both understanding the sources of cosmic rays through their interactions and learning from high-energy cosmic rays about fundamental particle properties – in particular, those concerning interactions at the highest energies, neutrino production and dark matter.

The three participating universities have a long tradition in investigating the aspects discussed above, with more than a decade of collaboration with each other across the three involved subdisciplines of physics. As an example, Technische Universität Dortmund joined forces with the Ruhr-Universität Bochum to contribute to the construction of the large-scale Cherenkov Telescope Array to investigate astrophysical processes. At the same time, researchers in Dortmund focus on developing statistical data evaluation methods, while those in Bochum model possible cosmic-ray astrophysical sources by using data from gamma and neutrino astronomy. For example, a multiwavelength model that predicts the simultaneous detection of gamma-ray signatures and cosmic ray ionization signals was developed at the Ruhr-Universität Bochum. Ionization processes are of fundamental relevance for the formation of larger dust grains in the Universe, leading to the formation of planets, which is studied at Universität Duisburg-Essen by Professor Wurm. Another example of the connection of the subdisciplines is the research of unit instabilities, turbulence, and transport in cosmic magnetic fields that principle investigators in Bochum have been studying over the past eight years, funded by the German Science Foundation. These examples show the long tradition of collaboration between the principle investigators at the boundary of the physics subdisciplines of plasma, astro- and particle physics. The foundation of the RAPP Center was a natural step to further enhance and foster these activities.

As Professor Tjus points out, the expertise available at the universities of Bochum, Dortmund, and Duisburg-Essen in the areas of particle, astro- and plasma physics is of high value towards finding answers to these important questions. Moreover, the technology required to explore these phenomena now finally exists. 'Traditionally, optical astronomy was, of course, the way to understand the Universe. Today, we have a large variety of frequencies that can be used to study distant galaxies or objects within the Milky Way, from radio wavelengths up to X-rays, and to even higher energies,' Professor Tjus explains. 'In astroparticle physics, information from cosmic rays, neutrinos, and high-energy photons is added to get a whole picture of the high-energy Universe. In the RAPP Center, we go even one step beyond this approach, trying to use fundamental physics input from basic research in plasma and particle physics in order to be able to explain the Universe from the lowest to the highest energies.'

As the first center in Germany where astro-, particle and plasma physicists join forces to understand cosmic interacting matter in the Universe, the RAPP Center hosted its first conference with over 100 participants in September 2016. As it stands today, the Center is an excellent choice for those who, like Professor Tjus and her colleagues, want the best of the three worlds: 'As a student, I was most interested in astrophysics and particle physics, so it was great not to have to choose between the two. In the recent years, I have learned how exciting plasma physics is and how important it is to explain our signatures. Yet, the combination of all these subdisciplines requires a large team of researchers already experienced in the topics in question – something that has developed naturally during the past decade through the collaboration of the different chairs involved in the RAPP Center. Just imagine, we try to describe particle interactions at the sub-nanometer scale, after they have propagated over millions of light years. These two worlds, the cosmological and the microscopic quantum world, cannot even be described by the same fundamental theory at this point, but it is still working quite well to combine them the way it's done in astroparticle physics. So far, it has often been neglected that the transport and interaction of these cosmic rays happen in a magnetized background plasma. During my time as a professor in Bochum I have learned how important this treatment is. However, the combination of all three research areas cannot be achieved by one single scientist. It requires the combination of experts from all of these disciplines. At the RAPP Center, we naturally host such an environment, in which 20 principle investigators have gathered to understand the signatures of interacting cosmic matters in the Universe.'

Group picture of RAPP Center members at the inauguration ceremony in September 2016

Meet the Researchers

Professor Julia Tjus

Professor Julia Tjus is the speaker of the RAPP Center and head of the Plasma Astroparticle Physics Group at Ruhr-Universität Bochum. She received her PhD in 2007 for her thesis entitled 'On the phenomenology of potential astrophysical neutrino sources', which was awarded the prize for the best thesis in physics at TU Dortmund that year. In 2013, she became a full professor and has since attracted numerous grants and awards for her work. As an example, she was awarded the Young Scientist Award of the International Union of Applied and Pure Physics (Section C4) in 2015. Her career currently follows both of her main research interests, namely the connection between astrophysics, plasma physics and particle physics. Her group is an active member of the IceCube and Cherenkov Telescope Array (CTA) collaborations.

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Professor Wolfgang Rhode, is the Co-Speaker of the RAPP Center and a professor at the Department of Physics at Technische Universität Dortmund (TU Dortmund). He received a PhD in philosophy in 1990 from the University of Freiburg and another one in physics in 1993 from the University of Wuppertal. He then continued his career in astroparticle physics. His main research interests are astroparticle physics, i.e. neutrino astronomy and gamma-ray astronomy, in addition to the utilization of computer science in physics and aspects of natural philosophy. Currently, he is involved in several national and international research collaborations, including IceCube and CTA.

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Professor Bernhard Spaan is a German research physicist and professor at TU Dortmund.He received his PhD in 1988 for his thesis on 'Investigations on rare decays of τ-leptons and on the mass of τ-neutrinos', which was awarded the Benno-Orenstein Prize in 1989. He continued his career in experimental particle physics with the experiments ARGUS, BaBar and now LHCb. In 1996, he joined Technische Universität Dresden as professor for experimental hadron physics. Since 2004, he has been full professor of experimental particle physics at TU Dortmund. Between 2008 and 2014, he was also dean of the Department of Physics of TU Dortmund.

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Professor Gerhard Wurm

Professor Gerhard Wurm is an astrophysicist and professor in the Department of Experimental Physics at Universität Duisburg-Essen. During his PhD studies, he joined a collaboration at the University of Jena, where he studied dust in star forming regions'. He continued his career at the University of Colorado, Boulder where he worked at the Laboratory for Atmospheric and Space Physics. Later on, he joined the Institute for Planetology of the University of Münster and finally joined Universität Duisburg-Essen in 2009.

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Professor Ralf-Jürgen Dettmar

Professor Ralf-Jürgen Dettmar has been a professor of astronomy at the Ruhr-Universität Bochum since 1994. In 1986, he received his PhD from the University of Bonn with a thesis project conducted at the Max-Planck-Institute for Radio Astronomy. Between 1986 and 1994, he was a postdoc at the University of Bonn, a fellow at Lowell Observatory in Flagstaff, AZ (USA), and worked for the European Space Agency (ESA) at the Space Telescope Science Institute in Baltimore. His research interests are centered on the evolution of galaxies and, more precisely, the interstellar medium in spiral galaxies.

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Professor Reinhard Schlickeiser

Professor Reinhard Schlickeiser is the Chair of the Theoretical Physics Department at Ruhr-Universität Bochum. He received his PhD from the Christian-Albrechts-University Kiel. After numerous collaborations with German and international universities, he became a full professor in 1998. Throughout his career, he has guided 36 PhD students to successfully complete their research and published almost 400 papers in peer reviewed journals, which have attracted over 22,000 citations. Out of all of his PhD students and postdocs, 15 are today permanent professors, research professors, or lecturers at universities worldwide. He is also an editor for four scientific journals and published a book titled 'Cosmic Ray Astrophysics'.

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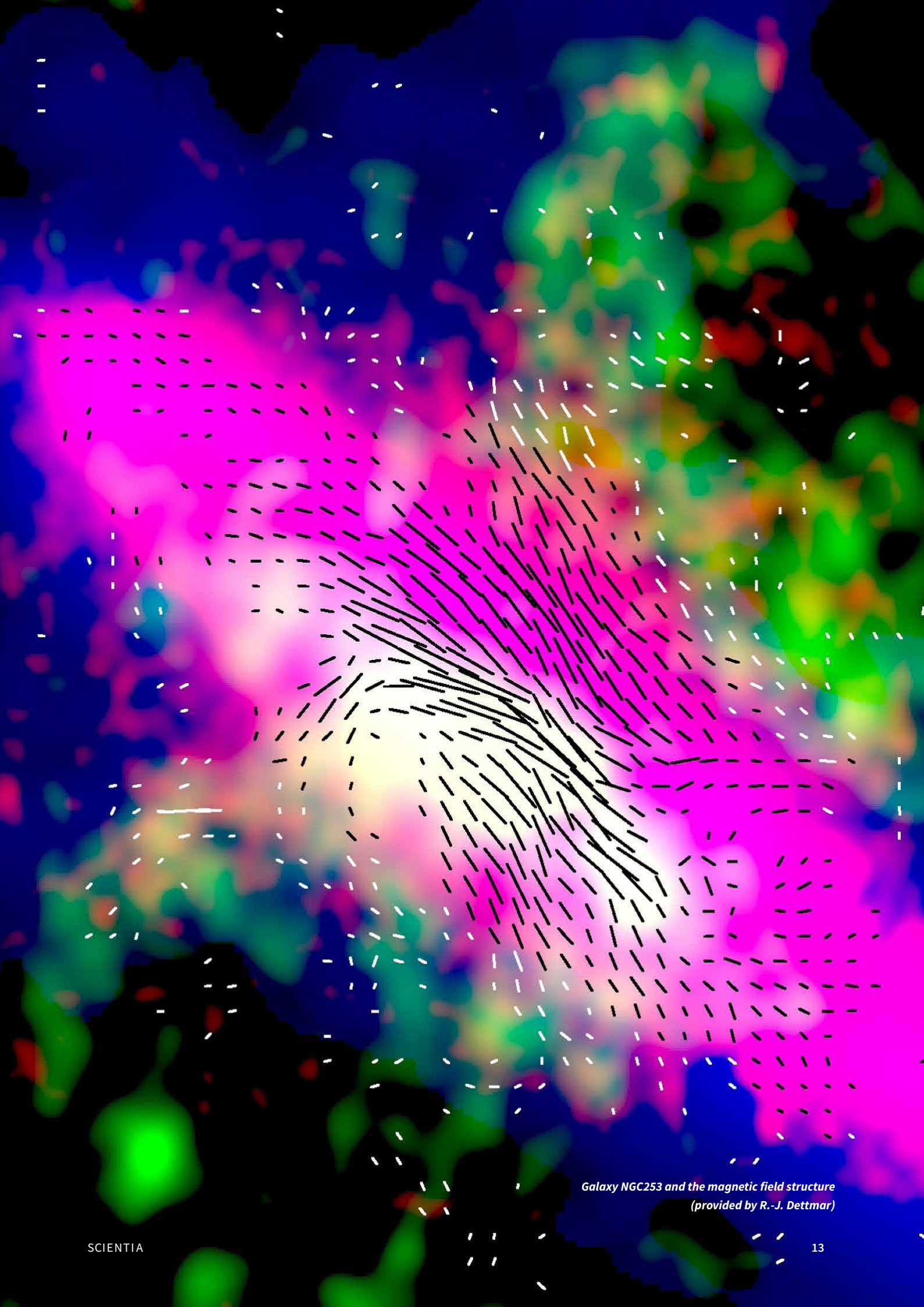
FUNDING

This brochure has been developed with the help of the Young Academy, Berlin, Germany. The RAPP Center is supported by the Mercator Research Center Ruhr (MERCUR).

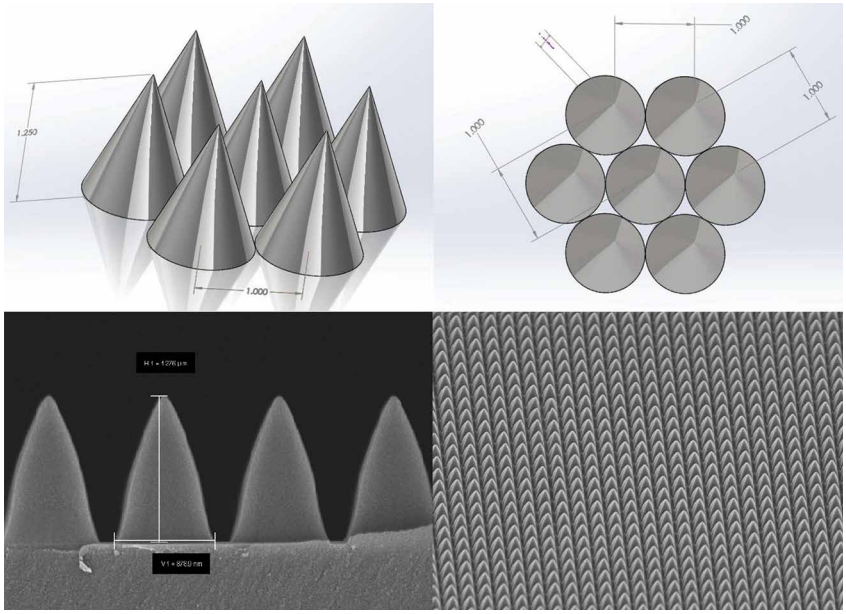
www.rapp-center.de



Galaxy NGC253 and the magnetic field structure (provided by R.-J. Dettmar)

TICAL AIMS FOR PARADIGM SHIFT IN PET IMAGING

In an ongoing effort to increase the accuracy and sensitivity of current PET (positron emission tomography) scanners, **Prof Paul Lecoq** and his team at CERN research various elements of this particular imaging technique. Inspired by particle physics detectors, the team is making ground-breaking modifications to current PET technology, which will help physicians make more precise diagnoses, implement more accurate treatment plans and increase patient survival rates for a multitude of conditions. From cancer and neurodegenerative conditions through to osteoarthritis and diabetes, all will see improved diagnoses and treatment regimens for an increased number of diseases and patients.



Photonic crystal: hexagonally close-packed array of nano-sized cones

PET as a Tool in the Fight Against Disease

Medical scanning technology has progressed swiftly over recent times. The implementation of various modalities such as magnetic resonance imaging (MRI), computed tomography (CT) and positron emission tomography (PET) has seen the medical sector enriched with many imaging techniques. These techniques have become essential tools in the early detection of many medical conditions, such as cancer, allowing for swift treatment and improved survival rates.

Because of its ability to study biochemical functions within the body, PET is often able to detect disease before the resulting changes in anatomy become apparent, making it a highly effective tool in diagnosing many diseases. However, one significant limitation of PET is that it exposes the body to radioactivity, making it unsuitable for use on children or pregnant women. Therefore, it is essential for research to improve the sensitivity of the technique so that radioactive doses can be reduced.

PET scanning works initially by injecting the patient with a substance called a radiotracer that homes in on the affected area. A specific radiotracer is selected for the patient depending on their disease and the body area to be scanned. In the case of cancer, this substance, similar to glucose, does not metabolise and accumulates in cancer cells, as they require more energy than normal cells for their fast and uncontrolled multiplication. Each radiotracer contains a radioactive element that constantly releases positively charged sub-atomic particles called positrons (the antimatter equivalent of electrons). When a positron meets an electron, both annihilate, releasing two oppositely directed gamma-ray photons. It is the role of the PET scanner to trace the path of these photons back to where they originated to isolate the disease centre.

The detectors contained within each PET scanner are in a 360-degree configuration surrounding the patient, so the constant flow of gamma rays from the annihilation events builds up a 3D picture of the diseased area. Physicians can then use these high-quality images to deliver treatments to their patients.

The major benefit of PET scanners over other imaging modalities is that it can directly measure complex metabolic processes, offering doctors the confidence to target highly critical molecular pathways of the activity of cells in different organs of the body, such as the brain or heart. While MRI can sometimes indirectly measure metabolic processes, it does so with poor sensitivity, at 'millimolar' or 'micromolar' concentrations. By comparison, current PET technology can analyse biochemical processes at the 'picomolar' level, making it over a million times more sensitive than MRI.

Improving Current PET Technology

To increase PET's sensitivity even further, researchers are attempting to achieve more precise timing information of the detected gamma-ray photons. This will allow a more detailed picture of the disease site to be obtained, through strongly enhancing the signal to noise ratio of the image. The so-called 'coincidence time resolution' (CTR) of a PET detector is the measure of how precise the timing information is. In current PET scanners, the CTR is approximately 500 picoseconds (or 500 trillionths of a second), which corresponds to an imprecision of 7.5 cm in the localisation of the event at the origin of the emission of the two gamma rays along the line of response (the line between the two corresponding detectors).

When photons are registered by detectors in a PET scanner, they are organised into time intervals, or time-bins. However, if the timing resolution is too low, uncorrelated particles are also collected within each interval, creating false readings. These spurious events create additional system noise and can corrupt potential image information. Fast CTR is therefore vitally important for medical imaging.

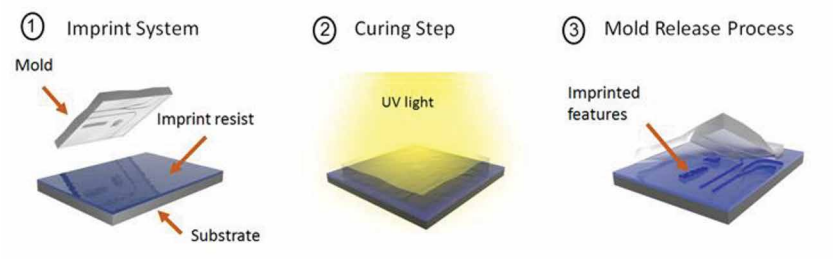
Although 500 picoseconds might seem fast in everyday terms, time resolution is an area that Professor Lecoq and his team in the Time Imaging CALorimeter project (TICAL) intend to improve. As Professor Lecoq highlights in a recent IEEE journal submission, this ambitious upgrade down to about 10 picoseconds is physically attainable, and will lead to vast improvements in image accuracy and signal-to-noise ratios. This is critical for improving the PET technique, as increased sensitivity will allow physicians to gather higher quality information faster and to reduce radiotracer doses, allowing in particular young children and even pregnant women to benefit from using PET.

Under a five-year European Research Council project, Professor Lecoq and his multinational team have been tasked to develop various aspects of the PET detection chain, from the optical materials responsible for detecting gamma rays, to the electronics that reads the converted electrical signals. Many aspects of the detection chain are responsible for timing delays, thus reducing the time resolution. For this reason, the entire five-year TICAL project has been broken down into several individual areas for investigation, with the primary purpose of reducing the time resolution to 10 picoseconds. This remarkable level of time resolution would be comparable to those achieved by particle physics detectors, such as those found at CERN.

Scintillation: Converting Light to Electrical Current

One key part of the detection process, where the magic happens, is the conversion of gamma rays into electrical signals. This is partly achieved by optical materials called 'scintillators' that are imbedded within the surrounding scanner (these materials are also used in particle physics detectors and have played a significant role in the discovery of the Higgs boson at CERN). When gamma-ray photons are absorbed by the atoms in a scintillator crystal, they become excited, causing them to emit light in a process known as fluorescence. This fluorescent light is then passed through a silicon-based photomultiplier (SiPM) where it is converted into an electrical current. Because scintillators play a pivotal role in the signal-conversion process, maximising how efficiently they can transport light is an important approach to improving PET imaging.

Scintillation materials come in many forms, from organic liquids, such as benzene, to gases and inorganic crystals. Because of its good performance and flexibility, Professor Lecoq and his team are concentrating their efforts on developing a metamaterial, combining the necessary high density (to allow gamma rays to efficiently interact) and good scintillation properties of lutetium



Schematic of the nanoimprinting process used for fabricating the photonic crystals

oxyothosilicate (LSO) with the ultrafast light emission of nano-scintillators made from zinc oxide or cadmium selenide. To date, the team's various techniques to improve the light output (amount of light released) from these LSO crystals have progressed well. This has primarily involved coating the scintillator's exit face – where light leaves to enter the SiPM – using nanoimprinting technology. These so-called 'photonic crystals' can be imprinted on several materials (preferably with a high refraction index), such as silicon nitride and titanium dioxide, onto the scintillator's surface.

Light bouncing around within scintillator crystals has been shown to be a significant area of time delay that inevitably reduces the light output efficiency. To aid this process, the TICAL team has developed an integrated computer simulation program. By integrating several job specific programs into one modelling platform, the researchers have been able to scrutinise important system variables such as light-ray direction and photonic crystal configurations. This has enabled the team to model specific photonic crystal coating geometries to maximise light output. The successful use of the team's innovative software scheme has already helped produce positive results, and in total, the team has not only increased the light efficiency output by 150%, but also significantly reduced the time it takes for the signal to be transported.

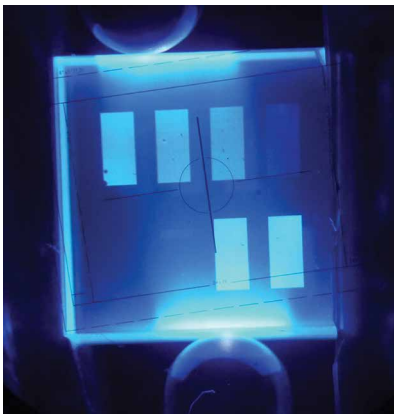
In conjunction with the advances made in the modelling software, the team has organised a collaboration with the Massachusetts Institute of Technology (MIT) and the companies Radiation Monitoring Devices and aBeam Technologies in USA, to develop a scalable and cost-effective production method for highly efficient photonic crystals. This has primarily involved engineering the individual photonic crystals into nano-sized cones.

As an additional research area, the team initiated the ULTIMA project to run in parallel with the TICAL project. This proof-of-concept project explores the use of engineered photonic crystals to boost the light output. When using their nanoimprinted photonic crystals, Professor Lecoq and the team have so far reported an increase in scintillated light output of greater than 40% and an increased energy resolution of up to 40% compared to currently-used non-coated scintillators. The team also highlights that, for commercial purposes, the process of nanoimprinting has been shown to be highly scalable as well as cost effective. ULTIMA has placed the project on a successful trajectory, as improved light output means a far superior image quality and hence a reduced need for high radioactive tracer doses prior to the scanning process.

Additional Developments and Future Applications

Under the overall management of Professor Lecoq, the entire TICAL project has been a coordinated effort between five individual teams of scientists from Fermilab in the US, the University of Bologna and CERN itself. All have been tasked to investigate additional areas of the detection chain with the ultimate goal of creating a highly accurate detector and reducing coincidence timing resolution to their target of 10 picoseconds.

This research will also have a multifunctional use, in that the team's detection materials will eventually also be integrated into future high-luminosity particle accelerators. Detectors (specifically called calorimeters) are used in particle physics to measure the energy of particle showers in atom smashing experiments. It is predicted that the research carried out by the TICAL and ULTIMA teams will be the initial steps on a path that will trigger a cascade of further research and development projects into PET imaging technologies. The hope is they will eventually



Enhanced scintillation light extraction from a UV-excited LSO crystal, on which six different photonic crystal patterns have been produced

crossover from academic research into everyday use, particularly within the medical sector.

Also, the researchers are working towards new advances in silicon-based photo-multipliers. Their new method, based on a silicon strip arrangement, backed up with improved readout capabilities, will help to bring the team's timing resolution ambitions within realistic view. The recently approved TWIST proof-of-concept project will run in parallel with TICAL and concentrate on the development of a PET module using this new photodetector technology.

PET was first introduced by David E. Kuhl of the University of Michigan in the 1950s, and has been in development under various guises ever since. However, as already mentioned, PET usage is currently restricted to the adult population. Over recent times, there have been many innovative advancements in medical imaging, from silicon based detectors used in proton beam scanners, to real-time near-infrared techniques to monitor malfunctioning lymphatic systems. Entering this pantheon of hi-tech innovation, TICAL and ULTIMA are working towards a paradigm shift in PET imaging systems, thereby widening its presently limited application. The team's ambitious goal to reduce the timing resolution to 10 picoseconds will increase the method's sensitivity, allowing doctors to reduce potentially harmful radiotracer doses, thus ensuring the technique becomes a truly universal diagnostic tool for future generations.

Meet the researcher

Professor Paul Lecoq
CERN
Geneva
Switzerland

Professor Paul Lecoq received his diploma in Engineering at the Ecole Polytechnique de Grenoble in 1972, under the leadership of Nobel Laureate Louis Néel. After two years of research at the Nuclear Physics Laboratory of the University of Montreal, Canada, he received his PhD in Nuclear Physics in 1974. Since then, he has worked at CERN on five major international particle physics experiments. He worked as the technical coordinator of the electromagnetic calorimeter of the CMS experiment at CERN, which played a vital role in the discovery of the Higgs boson. Prof Lecoq is also the founder of the CERN-based international Crystal-Clear collaboration, a group of 28 institutes and companies worldwide contributing to the development of scintillator science. He created the SCINT conference series in 1992, which gathers scientists who work on the fundamental aspects, production technologies and applications of scintillators. He is a member of a number of advisory committees and of international Societies, and was the promoter of the CERIMED initiative (European Center for Research in Medical Imaging, inaugurated in Marseille in 2014) in 2002 for networking physics and medicine in the field of medical imaging. In 2008, Prof Lecoq was elected a member of the European Academy of Sciences and in 2017, he was made Head of the Physics division of the Academy. In 2015, he was elevated to the status of fellow at IEEE – the world's largest technical professional organisation for the advancement of technology.

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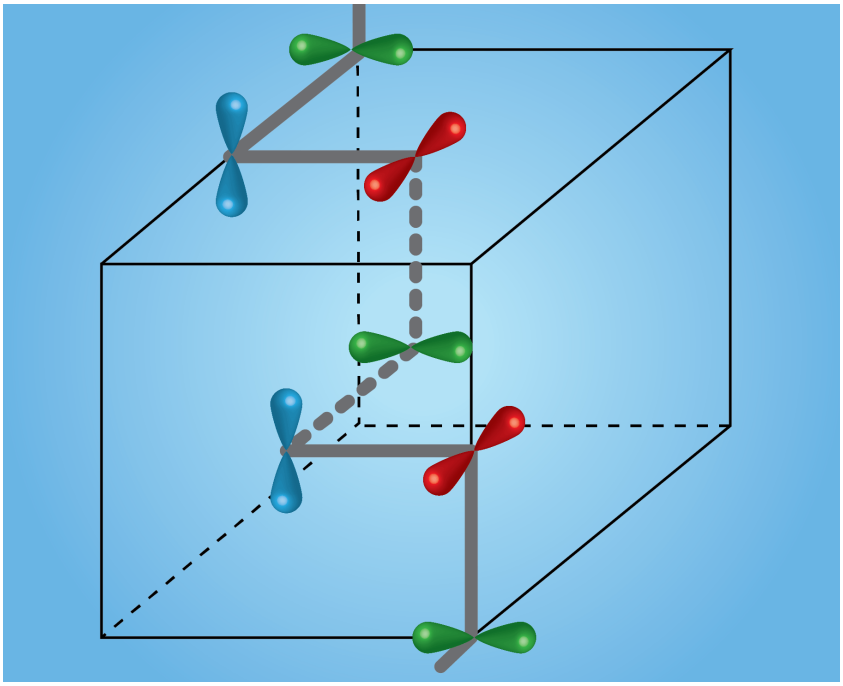
WP3: Light transport and photodetection optimization: Stefan Gundacker (CERN, Univ. Milano Bicocca), Matteo Salomoni (Univ. Milano Bicocca), Rosalinde Pots (RWTH Aachen, CERN), Arno Knapitsch (CERN)
WP4: Photodetectors and fast electronics: Crispin Williams (INFN Bologna, CERN), Katayoun Doroud (CERN)
WP5: 4D Calorimeter proof of concept: Tiziano Camporesi (CERN), Marco Lucchini (Univ. Milano Bicocca, CERN)

FUNDING

European Research Council, ERC Advanced Grant #338953

THE UNEXPECTED SPIRALS OF ELECTRON DENSITY

Spirals are an intriguing shape to find in the natural world because they have handedness – turning either to the left or right as you move along them – and it's this property that makes the work of **Dr Jasper van Wezel** and his team at the University of Amsterdam particularly interesting. The recent discovery that electrons within the material Titanium-diselenide can spontaneously form into a corkscrew shape was an unexpected example of a spiral emerging in physics – and Dr van Wezel and his colleagues have dedicated the past few years to developing a simple, yet eloquent explanation.



Understanding Atomic Structure

When atoms form into solids, their structure is dictated by where their electrons sit in the space surrounding the nucleus. This space is divided into electron 'orbits' – regions of space that can each hold a fixed number of electrons. As we move through the periodic table, from the lighter elements to heavier ones, the number of electrons each atom contains rises, and their orbits fill up in a well-defined fashion. The orbit closest to the nucleus holds the least number of electrons and, as we travel away from the centre, each orbit has a higher capacity than the last.

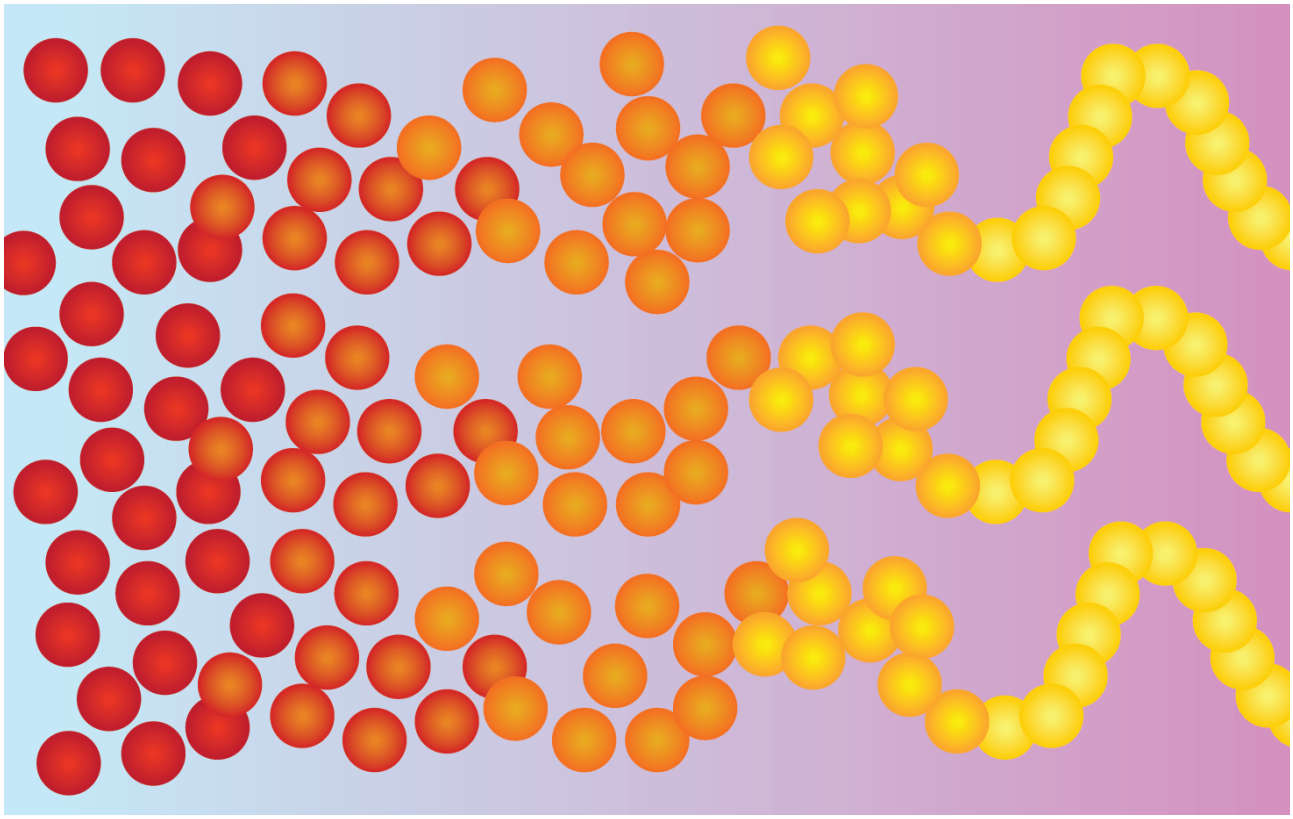
The electrons in the outermost orbits (the valence shell) dictate the chemical properties of an atom – if this orbit is completely full then the atom has a very low chemical reactivity and belongs to a group of elements known as the Noble Gases. Atoms with outer orbits that are not full can group together with other atoms to form molecules or crystalline materials. In a way, we can think of atoms joining together as jigsaw pieces – atoms with two electrons in their outer orbits will bond perfectly with atoms that are two electrons short of having a full orbit. But even if some electrons are 'left over' after bonding has taken place, these can be smeared out over the atoms in a crystalline material like an additional glue, resulting in crystals that conduct electricity.

When atoms bond together to form a material, they fall into a variety of ordered patterns and structures – from simple cubic shapes (where atoms occupy the corners of a cube) to hexagonal arrangements that resemble three-dimensional honeycomb structures. Many such structures are said to have an 'inversion symmetry', meaning that the atomic arrangement looks exactly the same if it is inverted, or turned inside out. In daily life, a plain T-shirt is an example of an object that has inversion symmetry, whereas gloves do not – you can wear your shirt inside-out as if nothing happened, but a right glove turned inside-out changes into a left one.

If a material is a metal, electrons normally float freely throughout the atomic structure in an 'electron sea'. These free-floating electrons are what gives metals their electrical current and heat carrying properties. Sometimes, though, they can break out of this sea and form structures of their own, which appear to be unrelated to the underlying atomic arrangement. Such a structure is known as a 'charge density wave', and can be thought of as a 'crystal' made up of electrons that coexists with the atomic crystal. In such situations, the electrons in the electron sea can no longer move freely – and the material becomes an insulator.

Charge density waves are an example of an 'emergent phenomenon' in physics. As explained by Dr van Wezel, 'Emergent phenomena occur regularly even in everyday life. For example, even though any two people will find it hard to applaud in the exact same

‘All of these properties of the charge density wave have a direct impact on the overall properties of the host material, such as its conductivity, the way it responds to light or applied electric and magnetic fields, and even the chemical reactivity of its surfaces.’



rhythm, a large audience at a popular Broadway play will spontaneously clap in harmony almost as soon as the curtain drops.’ In a similar fashion, a small number of electrons might not be able to escape existing in a disordered state, but the large numbers contained within even the tiniest amount of a solid material will, in the right circumstances, be able to collectively organise into an ordered arrangement in some places.

Electronic Spirals

Charge density waves are one of the most fundamental examples of an emergent phenomenon, yet they can still take on countless arrangements – with new structures being discovered even today. In 2010, Dr Junya Ishioka and colleagues at Hokkaido University in Japan demonstrated, for the first time, that charge density waves within Titanium-diselenide ($TiSe_2$) could spontaneously form into spiral structures. This discovery took physicists by surprise, as there doesn’t seem to be anything about electronic charge that can ‘rotate’ as you go along the axis of a spiral – the charge of an electron is just a number, not a shape that can be rotated.

‘Although spins, the arrow-like magnetic moments of electrons, are often found to arrange spontaneously into spiral magnetic structures, the electron charge has no in-built direction that can be varied in such a way as to create a spiral,’ Dr van Wezel explains. The spontaneous formation of spirals breaks the inversion symmetry of the structure, meaning that the charge density waves develop a property called ‘chirality’ – the structure and its mirror image cannot be superimposed, just like a right glove isn’t the same as a left one. Like most elegant theories, the solution to this particular problem turned out to actually be rather simple.

Pushing the Boundaries of Our Understanding

In 1913, Niels Bohr and Ernest Rutherford, the fathers of atomic physics, suggested that electrons orbiting an atomic nucleus can be modelled in a similar manner to the planets orbiting the sun – small, solid, planet-like balls circle around a much larger spherical object. Our most up-to-date models, however, tell a rather different story: ‘Electrons in free space are generally described as point particles. But when they are embedded within a regular atomic array, the electrons are actually better thought of as extended clouds. Some electron clouds are round like beach balls, others elongated like cigars, and some resemble the petals of a four-leaved clover,’ says Dr van Wezel. These ‘electron clouds’ are in fact nothing other than the valence (outermost) orbits mentioned before, and since they occupy a particular shape in three-dimensional space, they can be rotated.

Starting from this very simple idea, Dr van Wezel and his team developed a model for explaining the spontaneous chirality of charge density waves. To understand this model, we first need to cast our minds back to the simple cubic structure formed by some atoms as they bond into a solid material. The cube in question repeats itself throughout the entire three-dimensional volume of the

material, with an atom at each and every corner. In an ideal situation, every cube is identical and the material is the same throughout. But as any experienced scientist will tell you – we do not live in an ideal world.

After the Big Bang and the 'explosion' of matter into existence, it's thought that all material was spread out across the entire universe in an ordered, homogeneous way. Luckily for us, small instabilities led to some particles bunching together, causing localised distortions in the ordered structure of matter and, ultimately, leading to the formation of stars and all life as we know it. In the case of Dr van Wezel's model, tiny distortions in the electronic structure result in three different charge density waves, each being established among electrons occupying similarly oriented orbitals on different atoms. The fixed relative orientations of orbitals in different charge density waves combine to give rise to the spiral structure observed experimentally by Dr Ishioka and colleagues.

The creation of multiple charge density waves when the orientations of the orbits containing the electrons are fixed not only implies that there are spiral chains of high electronic density running through the material, but also that the particular orbits making up the structure rotate as you move along the spiral. As any emergent phenomenon, the formation of spiral charge density waves can only happen spontaneously as large numbers of electrons interact within a single piece of matter.

In 2010 and 2011, Dr van Wezel and his colleagues published their model in the journals *Physics* and *Europhysics Letters*, showing how the spiral charge order is formed and predicting that it is necessarily associated with a spiral arrangement of the electronic orbits. A further publication in *Physical Review Letters* in 2013 provided experimental verification of the proposed model and demonstrated the validity of the team's work.

Towards the Future

The presence of electron charge density waves that break out of their underlying atomic structure is a well understood phenomenon in physics. Dr van Wezel describes how this phenomenon can be exploited: 'All of these properties of the charge density wave have a direct impact on the overall properties of the host material, such as its conductivity, the way it responds to light or applied electric and magnetic fields, and even the chemical reactivity of its surfaces.' They have already been employed to create electronic switches, computer memory, optical filters and many other devices with important technological applications.

The discovery of this new spiral-shaped charge density wave has the potential to increase our control over such devices. 'Flipping the handedness of a certain material by some means may allow you to control the way in which it transmits circularly polarised light, or the way in which it conducts electricity, or perhaps even the way in which molecules with a given handedness can react chemically on its surface,' says Dr van Wezel. In principle, there is no telling how this phenomenon can change the way our devices interact with the world. It has already changed the way we understand the electronic structure of materials.

What's next for Dr van Wezel and his team? 'Although the study of spiral charge order started off with its experimental discovery in a particular material, the actual three-dimensional spirals of charge density have not been directly observed yet. Only indirect evidence indicates that they must exist,' he states. Direct observation is difficult, as spirals often form in small patches of right-handed and left-handed patterns. When these patches form close together, they can have the net effect of cancelling each other out. Most experiments are unable to focus down to a small enough patch and directly observe the spirals. Dr van Wezel and his team are currently in the final stages of putting together a more detailed model that could show us how to overcome this issue.

Spirals have captivated human beings for as long as we have had the means of recording our thoughts and feelings – we see them in prehistoric cave paintings, on the walls of Celtic tombs, and even in the work of famous artists, like Vincent van Gogh and The Starry Night. They appear throughout nature in often unexpected places and have attracted the attention of some of our most famous mathematicians – Fibonacci, Archimedes, Euler and Fermat, to name a few. The discovery of spiral-shaped patterns of electrons has uncovered a type of chirality in materials that was not previously understood, and opens the door for studying and employing them in as yet unknown ways.

Meet the researcher

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Dr Jasper van Wezel obtained his PhD in Theoretical Condensed Matter Physics from Leiden University. After graduating in 2007, he joined the University of Cambridge as a junior research fellow, where he began his research into the theory of charge and orbital order. On leaving Cambridge, he spent time in Argonne National Laboratory (USA) and the University of Bristol (UK). In 2014, he returned to the Netherlands as an Assistant Professor in Condensed Matter Theory at the University of Amsterdam and, since 2016, has been an Associate Professor in Condensed Matter Theory at the University of Amsterdam as well as an associate fellow of Homerton college at the University of Cambridge. Dr van Wezel also holds advanced teaching qualifications in both the UK and The Netherlands. Although interested in all aspects of Condensed Matter Theory, a large part of his recent focus has been on exotic types of charge and orbital order.

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FUNDING

Recent work is supported by a VIDI grant of the Netherlands Organisation for Scientific Research (NWO).

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University of Amsterdam

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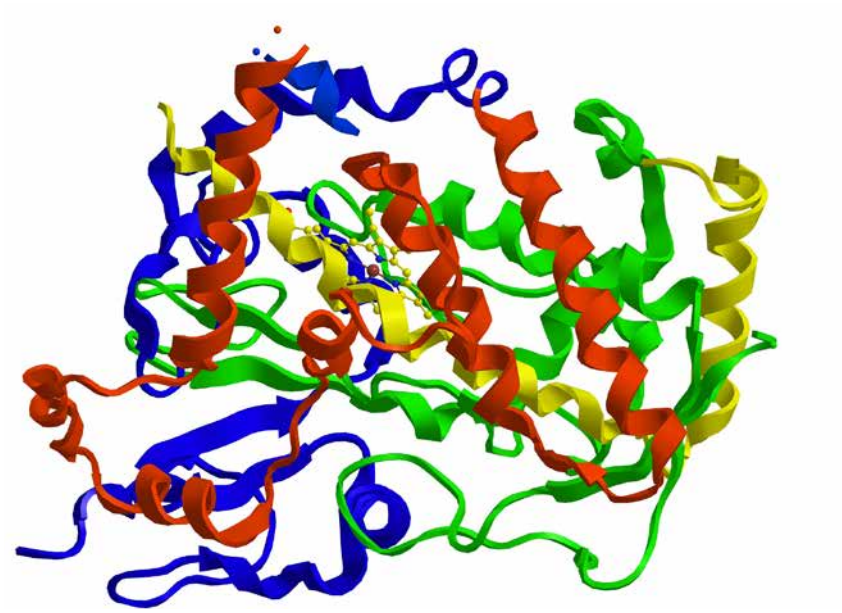
CALLING IN THE BIOELECTRICIAN

In the world of chemistry, the search for new and improved catalysts is of great importance. Inspired by a family of vital biological molecules, cytochrome P450 catalysts could be the way of the future for industry – if only they could be made to work better. **Dr Andrew K. Udit** and his team at Occidental College think they may be on the right track.



Our modern world is built upon chemistry – from the paint on our houses to our toothpaste containers, everything we use is supported by a vast industry that turns out millions of tonnes of chemicals we can barely pronounce, let alone identify. It is an industry where output is measured by the tonne and the megalitre, and where increasing efficiency by a fraction of a percent can boost profits by hundreds of thousands of dollars.

In order to maximise efficiency in the chemical industry, engineers and scientists must develop new processes to produce the required compounds and new catalysts to speed these processes up. Catalysts – often metal-based molecules – are able to increase the speed of a chemical reaction without being used up in the reaction themselves. This increase in speed can be the difference between a chemical synthesis taking minutes or taking centuries, and so research into new catalysts is a hot field for academia and industry alike.

Yet current catalysts have drawbacks – they are often expensive, toxic, and the reactions may still require strenuous conditions such as high temperatures or highly acidic environments. This has led to a broad search for new prospects, eventually leading all the way to the local biochemistry department, where a few scientists were working on a fascinating group of protein molecules known as the cytochrome P450 enzymes.

The Ubiquitous Family

The Cytochrome P450 family is a large group of enzymes found in every kingdom of life, from humans to mushrooms, and from plants to bacteria. First discovered in 1960, scientists have identified more than 18,000 different variants to date. As you would expect from such a large family, these enzymes play a number of different roles in the body. However, they are first and foremost catalysts – molecules that speed up chemical reactions. The most common of these reactions involves oxidation, whereby an oxygen atom is added onto a target molecule, known as a substrate.

These reactions generally involve the transfer of electrons to the enzyme from an external source. P450 enzymes consist of an iron-containing 'haem' molecule (which is also found in haemoglobin, the protein that carries oxygen around your bloodstream). This iron atom at the centre of the P450 enzyme picks up electrons and uses them to attract and capture oxygen atoms. As there are many different P450 enzymes, each with a different substrate that they work upon, a single molecule that enters the cell may be passed along from one enzyme to the next and eventually emerge as something completely different.
This modification, or 'metabolism', of molecules is extremely important for people who develop medicines, because almost 90% of all drugs will be changed in some way by P450 enzymes in the body. Scientists often use this to their advantage, designing molecules that are inactive when injected but become active once they are metabolised by P450 enzymes.

However, these enzymes are not only important for pharmaceutical companies – chemical manufacturers have taken note as well. Several P450 enzymes are able to catalyse industrially important reactions, turning fairly boring hydrocarbons into more complex molecules that can be used to produce new and exciting fuels, plastics, or drugs. More

‘Our ultimate aim is to develop a system that uses cytochrome P450 enzymes for medical and industrial use.’

importantly, many P450 enzymes do this in a fast, highly efficient, and extremely specific way – a far cry from the harsh conditions and inefficient transformations that can result when using other, traditional means.

Thus, P450 catalysts could be the way of the future for industry – if only they could be made to work better.

An Idea Whose Time May Come

Unfortunately, P450 enzymes have several disadvantages that prevent them from reaching their full potential in the industrial world, in particular their complexity, their cost, and the difficulty associated with working with large amounts of them (known in the industrial world as ‘scalability’).

Many of these problems come from the simple fact that P450 enzymes need electrons to do their work. In the cell, this is provided by an amazingly complex chain of reactions that eventually leads to production of an energy-carrying molecule known as NAD(P)H. Trying to reproduce this in the real world is vastly expensive, costing thousands of dollars per gram of product. Instead, researchers can try to supply the electrons directly, as electricity.

By sticking the P450 enzyme to a conductive surface, it is possible to supply a continuous flow of electricity (i.e. moving electrons) to the surface, and thus, the enzyme itself. In theory, the enzyme-coated surface could then continuously catalyse the chemical reaction of choice, quickly and efficiently, with no time needed to wait for the next NAD(P)H to come along. In practice, this is much more difficult than it sounds, because actually getting that electron to jump from the metal surface onto the iron atom of the haem molecule is quite complex. Scientists have had some success by genetically modifying enzymes or using techniques such as attaching tiny fat globules to gold wires – but results so far have not been impressive. There has been even less success for those working with bacterial P450 enzymes – usually considered more useful due to their robustness, speed, and ease of manufacture.

This leaves scientists with a problem. The potential uses for P450 enzymes are immense – but this potential can only be realised if the science can actually get to that point. Dr Andrew K. Udit and his team at Occidental College, Los Angeles, are working to solve these problems.

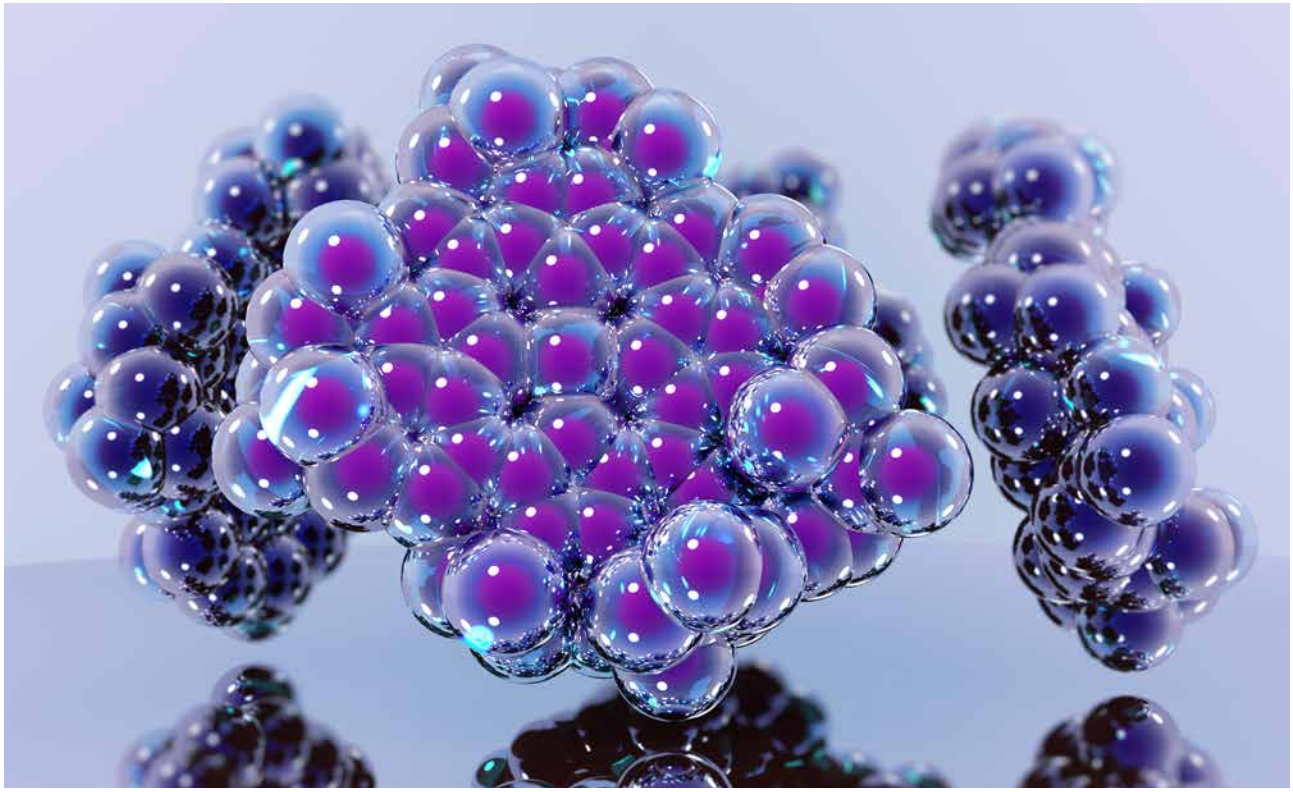
The Bioelectrician

An Associate Professor in the Department of Chemistry, Dr Udit’s work revolves around understanding and manipulating the activity of cytochrome P450 enzymes, especially when bound to metal electrodes. His team’s work to date has focused on the electrochemistry of P450 enzymes – the exact manner in which they use energy and electrons to power their chemical reactions. From here, they used their knowledge to study the enzyme-electrode processes, with the ultimate goal of tuning and controlling the enzymes themselves.

‘Our ultimate aim is to develop a system that uses cytochrome P450 enzymes for medical and industrial use,’ says Dr Udit. ‘The enzymes require electrons – “bioelectricity” – to run, which is hard to reproduce outside a living organism. We are trying to accomplish this by using an electrode to provide the necessary electrons.’

His team’s research has been split amongst three main goals: understanding the activity of P450-detergent films, running P450 reactions ‘backwards’, and improving electron transfer by identifying hot spots.

The team uses specialised techniques to coat P450 enzymes onto electrodes, most notably using a thin layer of detergent on top of a carbon electrode. This helps to boost the transfer of electrons between electrode and enzyme, which should improve the speed



of the catalytic reaction. Much of this depends on the specifics of the chemicals used, in particular the exact formulation of the detergent – certain detergent layers can make the enzyme unstable, potentially rendering it inactive. The team's further experiments will hopefully build on these findings and identify 'useful' detergent layers – those that stabilise the P450 catalyst, thereby improving its activity.

The second strand of Dr Udit's project involves reversing the normal catalytic cycle of a P450 reaction. In nature, P450 breaks apart a molecule of dioxygen (O_2) – one oxygen atom attaches to the central iron atom and is then passed on to the substrate molecule, while the other becomes bonded to two hydrogen atoms and goes floating off as water (H_2O). Normally, these dioxygen molecules are dissolved in water, which means that the industrial-scale catalytic reaction needs to be well aerated to work. However, it may also be possible to produce the oxygen required for the reaction by removing electrons from a water molecule bound to the haem iron in P450. Can this be used to produce the oxygen required by the P450 enzyme, thus avoiding the need to aerate the mixture? Dr Udit and his collaborators have been attempting to achieve this by carefully tuning the electrode/detergent surfaces and even mutating the enzyme itself.

The last part of the project revolves around identifying 'hot spots' for electron transfer – parts of the enzyme that are well suited for receiving electrons from the electrode. The team has come up with many techniques for attaching P450 enzymes to the electrode, including the use of molecular-scale wires such as pyrene.

Choosing the best place on the P450 molecule to make contact with this wire requires detailed knowledge about the surface of the enzyme and its capability for electron transfer. Towards this aim, Dr Udit's team 'mapped' the enzyme using a combination of atomic force microscopy and clever mutation of the enzyme's structure. Their work showed that the attachment point of the wire could significantly change the rate of electron transfer within the enzyme, which in turn strongly affected the overall catalytic ability. Based on these results, Dr Udit and his group intend to develop engineered enzymes with optimised electron transfer properties, further improving their performance for industrial settings.

Science for All

In addition to his research, Dr Udit is also actively engaged in several scientific outreach projects at Occidental College, one of the most culturally and economically diverse Liberal Arts colleges in the country. This includes several summer fellowships for undergraduates – an excellent way for those students to get a taste for research. He also teaches two outreach courses to first year students, one is a writing class called 'Science and You', the other is called 'Experiencing Mathematics and Science' (https://www.oxy.edu/core-program/fall-semester).

Catalysing the Future

Dr Udit and his team hope to further their understanding of the mechanism by which cytochrome P450 enzymes function, and use this knowledge to design even more effective variants. 'We have systems in place that can deliver the electrons,' comments Dr Udit, 'but the enzymes do not perform their natural function. The question is: why? Having solved the "bioelectricity" problem, our goal is to now determine what it will take to recover the enzyme's natural activity.'

Developing such an enzyme for 'green' industrial catalysis is a dream goal for many researchers in the field of chemical synthesis – and scientists such as Dr Udit are bringing this goal closer with each passing day.

Meet the researcher

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Dr Udit achieved his PhD in Chemistry with a focus on biocatalysis from the California Institute of Technology in 2005. After receiving his PhD, he worked as a Howard Hughes Medical Institute teaching-research fellow at Occidental College in Los Angeles. He then worked for two years at The Scripps Research Institute under a Canadian Institutes of Health Research fellowship studying bioconjugation methods, before returning to Occidental in 2008, where he is now an Associate Professor of Chemistry. Dr Udit has received several prestigious awards including start-up grants from the American Chemical Society Petroleum Research Fund, and the Camille and Henry Dreyfus Foundation. His high-quality work at the intersection of chemistry and biology has led to over 30 published papers, a patent, and numerous conference presentations. His education and outreach efforts have also been impressive – he has developed undergraduate courses, published several articles in newspapers, and acted as a mentor for more than 50 students.

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FUNDING

The National Science Foundation
The Research Corporation
The American Chemical Society Petroleum Research Fund
The Camille and Henry Dreyfus Foundation

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THE EXACTING TASK OF BRINGING MOLECULES TO ATTENTION

Molecules are relentlessly dynamic – vibrating, cartwheeling, and zig-zagging in a restless hustle. In order to study molecular properties and interactions, their motions must be tamed to a certain degree. In particular, the ability to make molecules face in a specific direction – to align or orient their axis – is sought in many diverse research areas. **Bretislav Friedrich** and his team at the Fritz Haber Institute, together with collaborators at Harvard, Purdue, Universität Regensburg, and the Freie Universität Berlin, have devised ways to coerce molecules into alignment and orientation. At the same time, they found exact solutions to the Schrödinger equation for particular strengths of the interactions between molecules and the electromagnetic fields that cause the aligning and orienting.

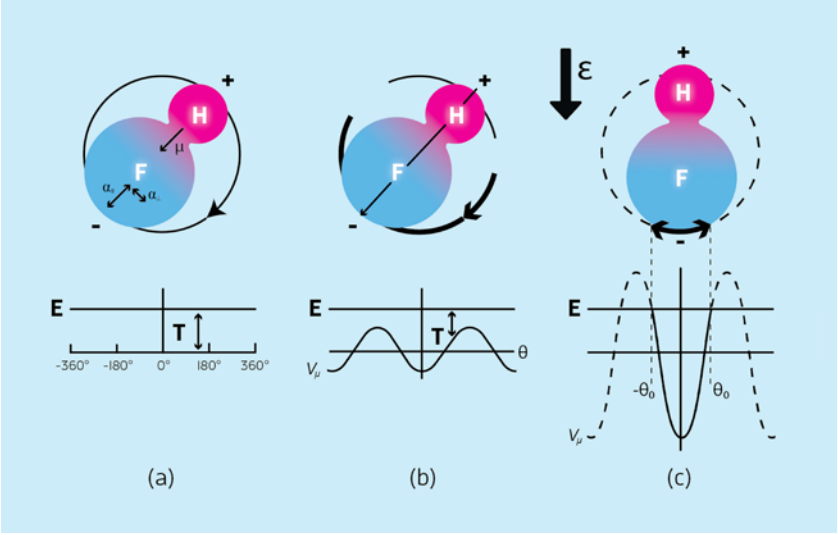

Figure 1

Oriented Molecules

It is often the case that the electrons that bind atoms into molecules are unevenly (anisotropically) distributed over the molecular frame. Think of a diatomic molecule such as hydrogen fluoride, HF. Because fluorine has a greater affinity (attraction) for electrons than hydrogen, the electron distribution is biased, with more (negative) electron charge concentrated on the fluorine atom than on the hydrogen atom. This makes the molecule polar, lending it a so-called permanent electric dipole moment (see Fig. 1). This dipole moment is fixed along the molecular axis that runs through the nuclei of the two atoms.

Since an electric dipole moment can be acted upon by an electric field (like a magnet can be acted upon by a magnetic field), the permanent, molecule-fixed electric dipole moment can be used as a lever to manipulate the molecular axis through its interaction with an external electric field. In the absence of the electric field, the dipole moment and thus the molecular axis is free to rotate in space (see Fig. 1a). When the electric field is turned on, the dipole moment is acted upon by the field proportionately to the dipole's magnitude, μ, the strength of the electric field, ε, and the cosine of the angle θ between the two. As a result, the energy of the electric dipole interaction becomes $V_\mu = -\mu\,\varepsilon\cos\theta$. Had the molecule rotated with kinetic energy T prior to switching on the field, its total energy in the field would then be $E = T + V_\mu$. If the total energy is to remain constant throughout the rotation of the molecule – as it should – the kinetic energy has to become dependent on the angle θ as well. As a result, the rotation in the field proceeds nonuniformly, but still covers the full range of 360° (see Fig. 1b).

The case of interest occurs when the permanent electric dipole interaction V_μ is cranked up so high that from some angle θ_0 on it exceeds the total energy E (see Fig. 1c). Then the kinetic energy is only nonzero (i.e., the molecular axis still moves) over an angular range that is less than 360°. This motion is called libration – an angular oscillation between the turning points at θ_0 defined by the intersection of E and V_μ, where the kinetic energy winds down to zero. One can see that in effect the molecular axis has become oriented along the direction of the electric field.

Since the to and fro motion is analogous to that of the pendulum (also defined by a cosine potential, between the bob's suspension and the gravitational field), the orientation achieved in this way is termed pendular orientation. We note that the kinetic energy

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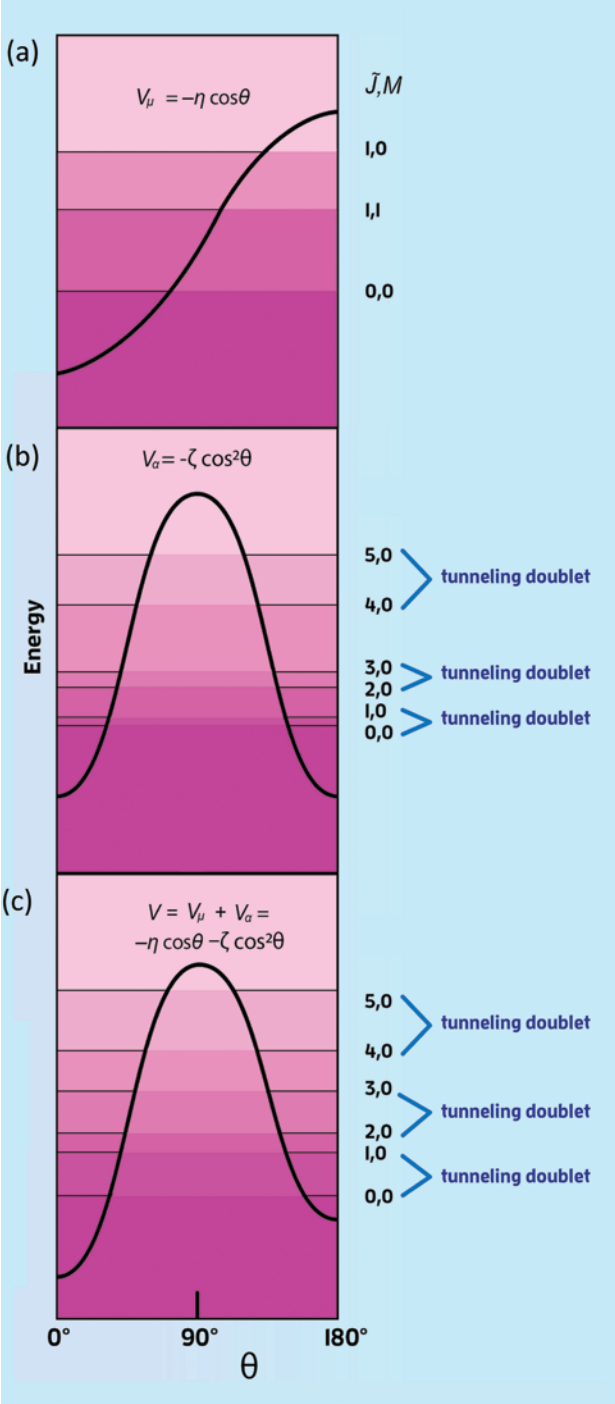


Figure 2

T of the molecule's rotation does not only depend on the amount of initial angular momentum (i.e., how fast it rotates) but also on the molecule's mass distribution, as captured by the quantity called the rotational constant, B. By dividing the permanent dipole interaction V_μ by the rotational constant we end up with a quantity V_μ/B that is independent of any particular (diatomic) molecule, as it contains all the molecule-specific parameters on which its motion – with a given angular momentum – in the electric field depends. We write $V_\mu/B = -\eta \cos\theta$, where $\eta = \mu\,\varepsilon/B$ is a dimensionless parameter – just a number – that fully characterises the strength of the orienting permanent dipole interaction of a polar molecule with an external electric field. One can immediately see that the orienting interaction will be strong for molecules with a large permanent dipole and low rotational constant (the latter possessed, roughly speaking, by heavy molecules). Not all molecules offer such properties, and therefore, pendular orientation is not as versatile as one would wish.

Molecules in Alignment

A dipole moment can be also induced in a molecule – whether polar or non-polar – by an external electric field. The induced dipole moment depends on the molecule's polarisability, which is a measure of how tightly the molecule's electrons are bound. The induced dipole moment can be then acted upon by the very electric field that has induced it. If the polarisability is uneven (anisotropic) over the molecular frame, the induced dipole moment is again molecule-fixed and can be used as a lever to manipulate the rotation of the molecule.

Because of the 'double action' of the electric field (inducing a dipole moment and then acting on it), the induced dipole interaction is proportional to its square as well as to the square of the cosine of the angle θ between the molecular axis and the direction of the field. It is also proportional to the polarisability anisotropy, $\Delta\alpha$, which, for the example of a linear molecule, is the difference between the polarisability parallel $\alpha_{\parallel}$ and perpendicular $\alpha_{\perp}$ to the molecular axis. Unlike the permanent body-fixed electric dipole moment, a single-headed arrow, the polarisability anisotropy is a double-headed arrow, since it does not distinguish, in our example, between the H and F atoms (see Fig. 1). Hence the induced dipole interaction can only align the molecular axis. It is given by $V_\alpha = -\Delta\alpha\,\varepsilon^2\cos^2\theta$ or, divided by the rotational constant of the molecule, $V_\alpha/B = -\zeta\cos^2\theta$, with $\zeta = \Delta\alpha\,\varepsilon^2/B$. Thus, the strength of the induced dipole, aligning interaction is universally characterised by the dimensionless parameter ζ, a number.

In order to make the alignment parameter (and hence the alignment attained) sizeable for typical molecules (say $\zeta > 10$), the electric field strength has to be raised to values that are too high to be attained in static electric fields (made by a high-voltage capacitor). Instead, the electric field of an intense electromagnetic wave produced by a laser has to be used. Such an optical field of intensity, I, gives rise to an electric field $\varepsilon_{opt} = (2I/c\epsilon_0)^{1/2}$, where c is the speed of light and ϵ_0 the vacuum permittivity. For instance, an optical field of an intensity of 10^{12} W/cm² produces an electric field ε_{opt}= 19,410 kV/cm, whereas a realistic maximum value of an electrostatic field is only about 100 kV/cm (i.e., about 200 times less). The requisite high optical intensities can only be achieved with pulsed lasers; however, the duration of the laser pulse can easily exceed the rotational period (h/2B, with h Planck's constant), in which case the optical field during the pulse behaves as if it were static at any moment.

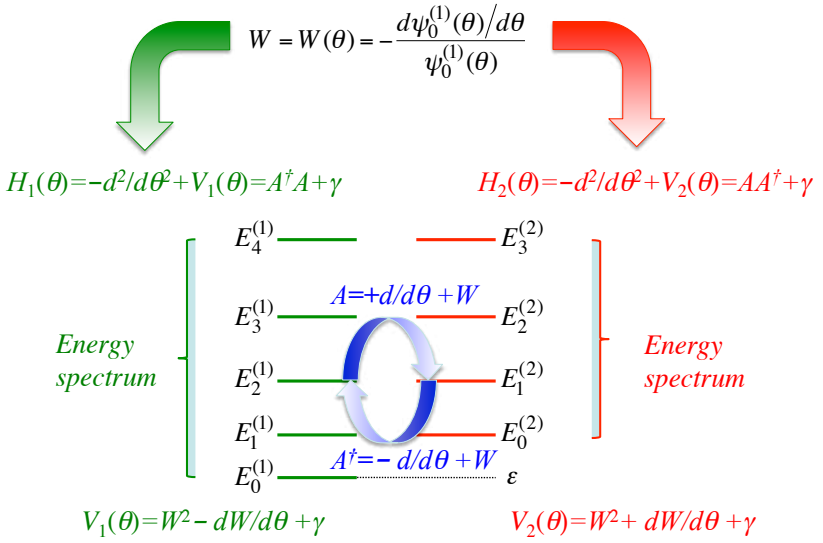


Figure 3

Enter Quantum Mechanics

The above description of the dynamics of a polar and/or polarisable molecule in an electric field draws on classical mechanics, as given, for example, by Newton's laws of motion. However, a molecule is a quantum-mechanical object that obeys the laws of quantum mechanics, as encapsulated, for example, in the Schrödinger equation. As famously pointed out by Paul Dirac, 'The underlying physical laws necessary for the mathematical theory of ... the whole of Chemistry [molecular science] are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations [Schrödinger's equation] that are too complex to be solved.'
There are a handful of problems in molecular science for which Schrödinger's equation can be solved (one speaks of an analytic or exact solution – which is just a closed-form formula that consists of elementary functions such as powers, trigonometric functions, etc.), such as the harmonic oscillator (a model of molecular vibration) or the hydrogen atom (a model of atomic shell structure). However, for the vast majority of problems, Schrödinger's equation can only be solved numerically, and moreover, usually after being simplified. The quantum pendulum problem (involving a molecule subject to a permanent and/or induced dipole interaction with an external electric field) belongs in the latter category – and can in general only be solved numerically (with arbitrary accuracy). These numerical solutions provide the energies as well as the wavefunctions of the various states that the molecule can have at given values of the parameters η and ζ (see Fig. 2).

A Versatile Recipe to Orient Molecules

As noted above, pendular orientation is only applicable to molecules with special properties. Therefore, a more general approach to orienting molecules was sought – and found – by Friedrich and his colleagues, using a technique based on the combination of a static electric field with a non-resonant optical field. The orientation occurs for any polar molecule, as only an anisotropic polarisability, along with a permanent dipole moment, is required. This is always available in polar molecules. Thus, for a great number of molecules in their rotational ground state, a static electric field can convert alignment by a laser into a strong orientation that projects up to 90% of the body-fixed dipole moment on the direction of the static field. Friedrich's 'combined fields' technique has been used in applications ranging from molecular imaging to surface science.

The strong orienting effect of the combined fields arises from the coupling of the members of the doublets generated by the induced-dipole interaction (the so-called tunnelling doublets, shown in Fig. 2b) by the permanent dipole interaction (shown in Fig. 2a). Fig. 2c shows the combined interaction along with the corresponding energy levels. One can see that adding the permanent dipole interaction makes the combined interaction asymmetric and draws the nearly degenerate (of nearly same energy) tunnelling doublets apart. Such a marked change in the energy of a given quantum state with the permanent dipole interaction is an unequivocal indication that the state in question has become highly oriented. We note that the combined fields effect is much more than the sum of its parts. This finding will be revisited below.

Analytic Solutions to Schrödinger's Equation for Molecules in Combined Fields

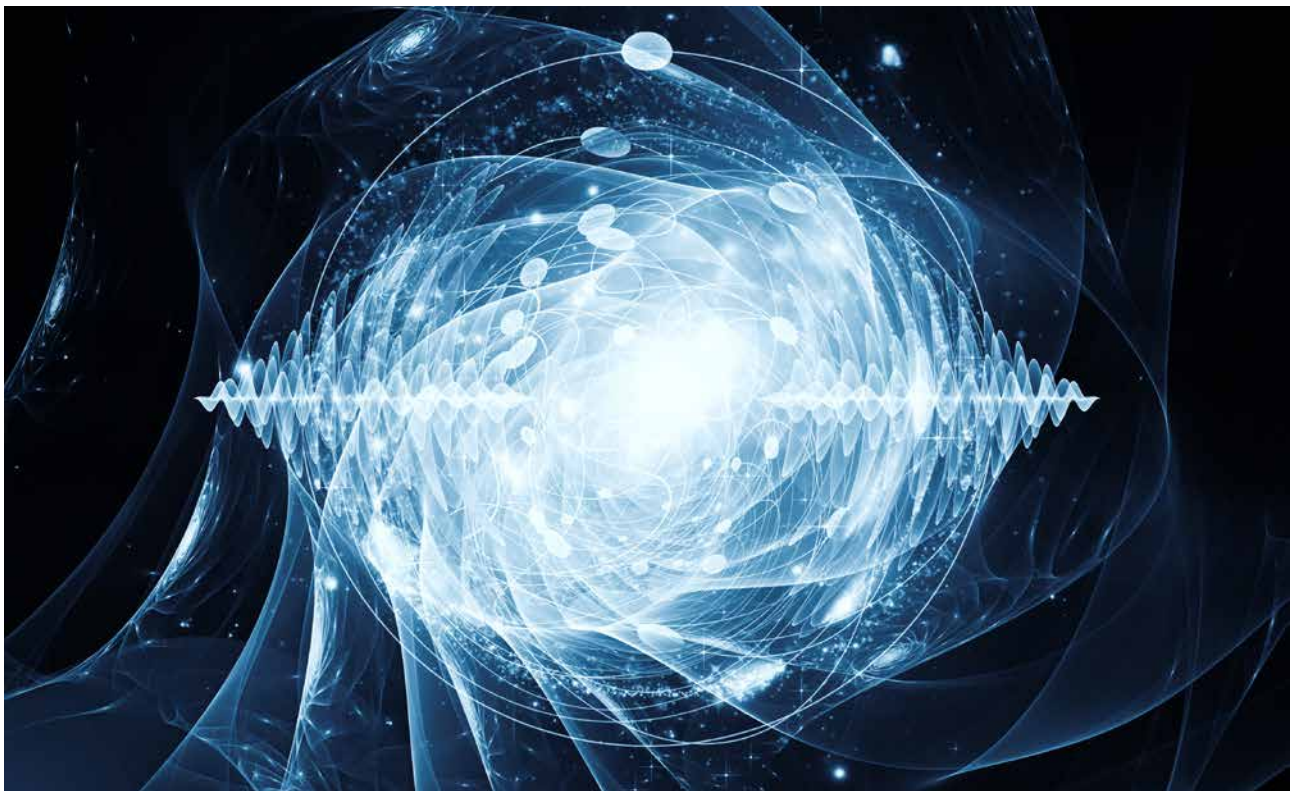
But what about any analytic solutions to the Schrödinger equation for a molecule in combined fields? 'Analytic – or exact – solutions are the gems of physics: beautiful and rare, furnishing an unrivalled insight into a problem's nature,' says Friedrich. 'It is a part of the culture of physics to seek them.'

The scarcity of analytic solutions to problems arising in quantum mechanics has not only spurred the development of techniques to find their numerical solutions instead, but has also impelled attempts to search for a type of analytic solution that only obtains for a subspace of the parameters that specify a given quantum mechanical problem. So, for instance, while the harmonic oscillator problem is analytically solvable for all values of the parameter on which it depends (the reduced force constant), the quantum pendulum one is not. Rather, the pendulum problem is only conditionally solvable, that is, its closed-form solutions only exist if the problem's interaction parameters satisfy a particular set of conditions. These are the orienting and aligning parameters that determine the interaction of a polar and polarisable molecule with an electric field (or a combination of an electrostatic with an optical field). Moreover, the analytic solutions only exist for finitely many states.

But how do we find the analytic solutions and the conditions under which they obtain?

Enter Supersymmetry

Supersymmetry was introduced as a presumed spacetime symmetry (relating fermionic and bosonic degrees of freedom) in search for physics beyond the so-called Standard Model of particle physics. Supersymmetry may not be corroborated by experiment any time soon – in fact, indirect evidence from the Large Hadron Collider



suggests that supersymmetry between fermions and bosons does not exist. However, this has no bearing whatsoever on the so-called supersymmetric quantum mechanics (SUSY QM).

SUSY QM was worked out in 1981 by Edward Witten as a model, with the goal of studying the structure and properties of the original spacetime SUSY. SUSY QM soon acquired a life of its own, which reached an early climax in 1983, when Lev Gendenshtein established a connection between SUSY as it arises in SUSY QM and analytic solvability. He showed that all known analytically solvable problems in quantum mechanics exhibit SUSY – and an additional property, called shape invariance, which is defined with the help of SUSY.

In what follows, we'll use the word supersymmetry or SUSY exclusively for supersymmetric quantum mechanics, which has meanwhile become well-ensconced within mathematical physics.

Supersymmetry, shown schematically in Fig. 3, is a relationship between two so called superpartner potentials, V_1 (green) and V_2 (red), both derivable from the same superpotential, W, and with states intertwined by the operator A. Now how do we solve the quantum pendulum problem with the help of SUSY? First, we make an Ansatz for the superpotential. That's the difficult part, like in integration by substitution. Once we have a viable Ansatz, such as $W = \alpha \cot\theta + ß \sin\theta$, the rest is easy. Then we set the pendulum's interaction potential equal to either V_1 or V_2, make use of the corresponding Ricatti equation, $V_{2,1} = W^2 \pm dW/d\theta + \gamma$, and determine the constants α, ß, and γ. From there we get the energy, E_0, and the corresponding wavefunction, ψ_0. However, since ß locks η and ζ to one another, we end up with a restriction on the ratio of the interaction parameters for which the analytic solutions obtain, namely $\zeta = \eta^2/4k^2$, where k = 1,2,3, … is an integer.

So far, Friedrich and his collaborators found a number of analytic solutions and identified conditions under which they obtain for both the full-fledged three-dimensional – spherical – pendulum (8 solutions) and the two-dimensional – planar – pendulum (40 solutions). Interestingly, no solutions were found for either a pure permanent dipole ($\zeta = 0$) or induced dipole interaction ($\eta = 0$).

In the course of their work, the researchers also investigated the dependence of the energy of the quantum pendulum on the interaction parameters η and ζ for its various quantum states. These energy surfaces (energy as a function of the two parameters η and ζ) were found to exhibit numerous intersections (see Fig. 4). Unsurprisingly, given that the tunneling splitting at fixed ζ increases with η, the upper member of the lower tunneling doublet is bound to meet the lower member of the upper tunneling doublet at some point. This then results in the observed pattern of intersections (all of them are so-called avoided intersections).

At this point, the researchers asked themselves whether the loci of the intersections (where the energy surfaces intersect) can be expressed analytically – and found that the answer is yes: the avoided crossings occur along parabolae given by the formula $\zeta = \eta^2/4k^2$, with k = 1,2,3, … an integer. But they had found this very formula already before: it is the condition for analytic solvability of the quantum pendulum problem! This is how the researchers realised that analytic solvability and the topology of the energy surfaces are closely connected. But what does exact solvability have to do with the topology of the energy surfaces? That's the one million-dollar question that the team is trying to answer in their ongoing work. A clue as to the origin of the magic connection comes from the structure of the matrix representation of the quantum pendulum problem.

Prospects

By also studying the two-dimensional planar pendulum, Friedrich and his team were inspired to find additional solutions to the three-dimensional pendulum problem. 'The planar case is quite instructive and in fact much of what we did on the full-fledged three-dimensional

pendulum we first practiced on the planar one,' he says. Equipped with many more analytic solutions in 2D, this search will continue. 'Moreover, the planar pendulum is related to an analytically solvable double-well problem.' The 'double-well' is another example of a quantum mechanical problem, which is also only conditionally analytically solvable. It involves two potential energy minima (or wells), which are separated by a barrier.

He goes on to say that, 'there are other potentials that occur in molecular quantum mechanics, such as the anharmonic oscillator, that we are set to explore as well.' An anharmonic oscillator (which, unlike a harmonic oscillator, has energy levels that are not equidistant) can model nuances of molecular vibration as well as other problems. As Friedrich says, 'in fact, the quantum pendulum is a sort of anharmonic oscillator', so he is looking to use his previous solutions to the quantum pendulum to explore the anharmonic oscillator in more depth.

A greater goal of all of this work is to clarify what SUSY and exact analytic solutions have to do with the energy surface topology described earlier. And last but not least, there's the supersymmetric Wentzel-Kramers-Brillouin (WKB) approximation that is of interest wherever WKB is of interest. WKB SUSY has already proved its worth explaining how the analytic form of the pendular ground state wavefunction comes about at an integer value of the topological index, thereby providing another clue as to the magic connection between analytic solvability and energy surface topology.

So, what are analytic solutions good for? In the first place, they can be used to evaluate, in analytic form, the characteristics of the strongly oriented and aligned molecular states that they pertain to. So apart from being beautiful and rare, these analytic solutions are also practical, for they allow to reverse-engineer the quantum problem and find the values of the parameters required for creating quantum states with preordained characteristics. The analytic solutions can also

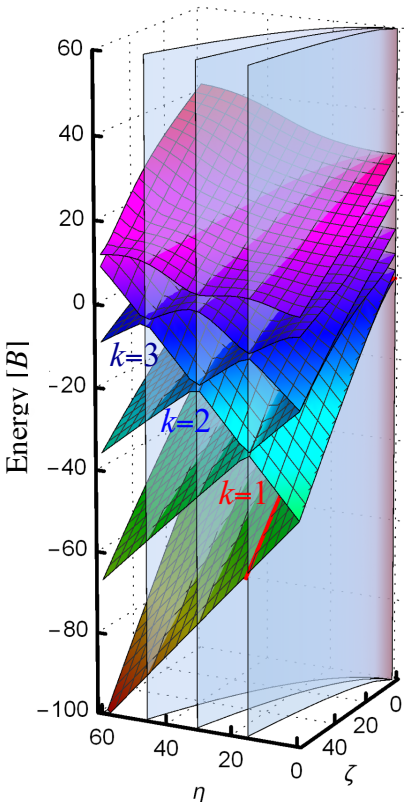


Figure 4

be used as benchmarks to check numerical calculations. Last but not least, the analytic solutions provide an insight into the workings of the quantum pendulum – or the Stark effect, in the case of a molecular realisation of the pendulum.

Meet the researcher

Professor Bretislav Friedrich

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Bretislav Friedrich was born in Prague, Czech Republic, and graduated from Charles University, in 1976, with a degree in physical chemistry. His diploma thesis dealt with non-ideal behavior of macro-molecular solutions in mixed solvents. Upon graduation, he switched fields to study the dynamics of ion-molecule reactions in crossed molecular beams at the J. Heyrovsky Institute of Physical Chemistry and Electrochemistry of the Czech Academy of Sciences, where he earned his PhD in 1981. Subsequently, he switched countries as well, more than once. He was an Alexander von Humboldt Fellow at the Max Planck Institute in Göttingen (1986–1987), Research Associate and later Senior Research Fellow and Lecturer at Harvard University (1987–2003), and, since 2003, a Research Group Leader at the Department of Molecular Physics at the Fritz Haber Institute of the Max Planck Society in Berlin. He is also an Honorary Professor at the Technical University of Berlin. Friedrich is world-renowned for his pioneering research on the interactions of molecules with and in electric, magnetic, and optical fields. Although his current research is chiefly theoretical, it is closely linked to ongoing experiments in a number of laboratories worldwide. Aside from his research, he maintains an abiding interest in the history of science (emergence of quantum mechanics, rise of physical and theoretical chemistry, scientific biography) and is engaged in efforts to eliminate chemical and other weapons of mass destruction.

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FUNDING

Max-Planck-Gesellschaft, Deutsche Forschungsgemeinschaft

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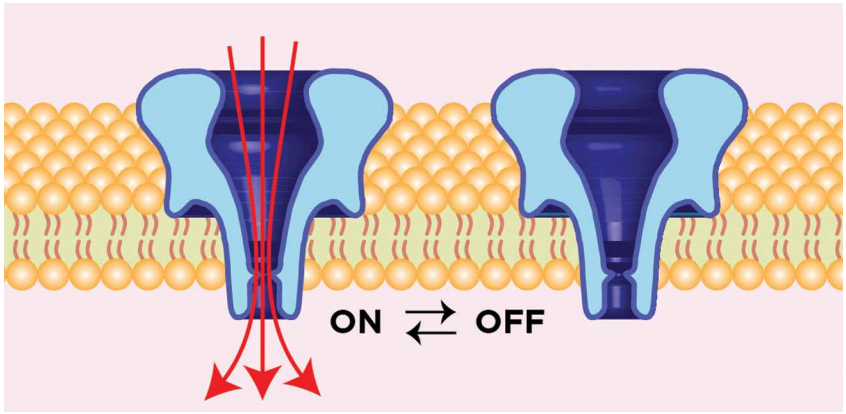
MONITORING AND CONTROLLING THE DELIVERY OF SINGLE MOLECULES THROUGH NANOPORES

Monitoring and controlling molecules as they are transported in and out of nanometre-sized compartments is no easy task. **Dr Lisa Burden, Dr Daniel Burden** and their colleagues at Wheaton College have made significant contributions to understanding these processes by developing nanoscale components inspired by cell membranes. They are also creating methods to interpret the signals that arise during transportation. These methods can be exquisitely sensitive, revealing even the tiniest signatures created by individual molecules.



Protein ion channels embedded within cell membranes offer a route for molecules to enter and exit the cells in our bodies. The biological purpose of these channels is to deliver and remove substances essential for many central life processes, including nerve signal propagation and protein synthesis. The type of molecule and how much it interacts with the walls of these ion channels allows our bodies to monitor and control many complex and intricate chemical reactions.

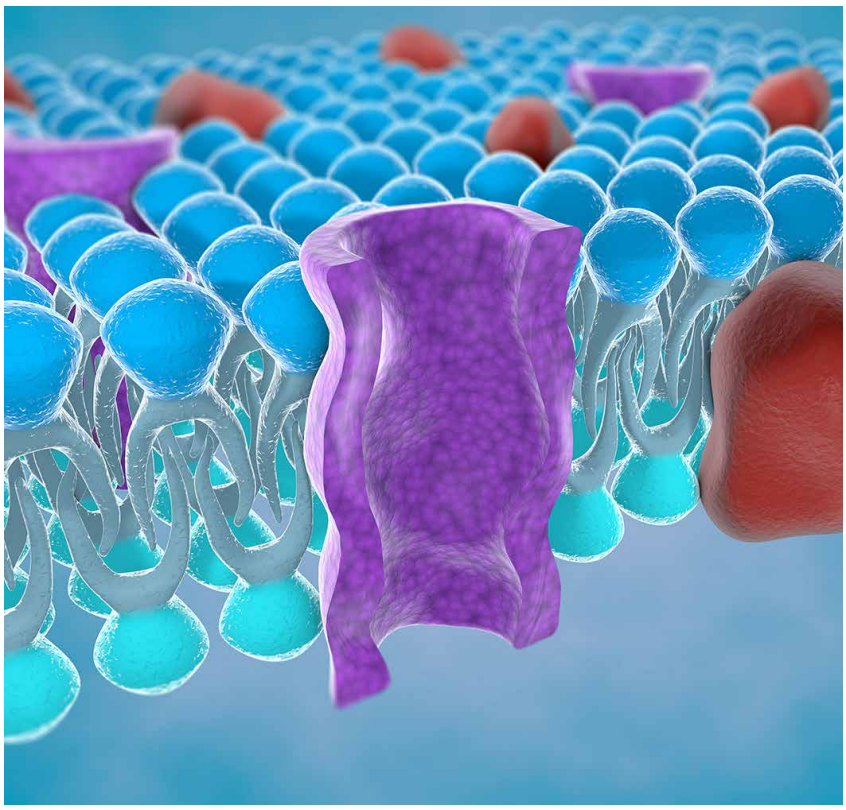
The question of how to observe and control these tiny molecular events in the macroscopic realm that is accessible to us presents a persistent challenge. If scientists could have complete control over molecular transport in and out of cells, then they could design efficient chemical sensors inspired by the properties of these membrane ion channels. Sensors based on cell membranes have a wide variety of applications in different fields, such as medical diagnostics, monitoring targeted drug delivery, determining the rate of cellular drug uptake, and even measuring environmental pollutants.

In a membrane-based sensor, these channels are typically called 'nanopores', which run transversely through a lipid membrane. To increase the probability that a nearby small molecule will pass through a nanopore to the other side of the membrane, an external voltage is applied. Once energised, the electrostatic attraction between the molecule and cell membrane promotes rapid molecular transport through the pore.

Dr Daniel Burden, Dr Lisa Burden and their colleagues at Wheaton College are focused on designing controllable membrane-based tools for the detection and delivery of small molecules that move between fluid-filled compartments. 'Our research attempts to harness existing cell-membrane proteins from a variety of microorganisms, understand their function, and implement strategies for chemical modification that will transform the protein from its native function to a desired chemical sensing, or transport control application,' explains Dr Lisa Burden.

Nanopore Sensors

To develop an efficient membrane-based sensor for DNA sequencing applications, the rate of interaction between moving molecules and the nanopore walls needs to be controlled. Towards this end, DNA chains that contain the genetic information can be labelled with additional molecules, such biotin (a small vitamin), fluorescent compounds that glow, or streptavidin (a protein that binds biotin). When biotin- or streptavidin-bound DNA approaches an ion channel, applying an external voltage can determine whether the DNA strand enters this channel or is driven away into the surrounding solution. When driven into the pore, the extra size of the attached label helps slow, or even stop, DNA transport. This makes the DNA easier to detect with electricity. By adding labels that glow, researchers can capitalise on secondary optical signatures that also characterise the transportation event. Together, both electrical and optical measurements yield more information about the nature of the DNA interaction with the



inner walls of the pore and can potentially unlock sequence information that is hidden within the DNA structure itself.

The Burden lab proposed a new method to simultaneously characterise the optical and electronic properties of a membrane-based sensor, taking advantage of the controllable behaviour of biotin- and streptavidin-bound DNA. Through the combined use of fluorescence microscopy and electrical current measurements, the team was able to quantify the electrical and optical signals associated with a fluorescently labelled DNA molecule and the nanopore.

When an external voltage is applied to the system, the distribution of electric charge (or polarity) on the membrane changes. This change in polarity then drives the labelled DNA strand to enter the channels. When the streptavidin-bound DNA enters a channel, the labelled molecule starts to fluoresce and the team can detect this fluorescence signal. If the DNA strand leaves the ion channel and goes back into the main solution, the fluorescence response is switched off and can no longer be detected. The correlation between the fluorescence activity and membrane polarity allows the team to calculate diffusion constants, which describe rates of molecular movement. This dual optical and electrical approach explored by Drs Lisa and Daniel Burden can also be used to study cellular processes at microsecond time resolution, thus allowing the scientists to directly observe and study the transportation of molecules into a cell.

Taking a Nanopore's Temperature

The 'potential energy surface' of a molecule describes the energy difference between its stable and unstable geometries. When the energy difference is less than the available thermal energy, temperature changes can reconfigure a molecule's shape in favour of high-energy (unstable) and more reactive geometries. To probe unstable geometries that occur quickly, these temperature changes need to take place very rapidly, with exact spatial precision, and in a way that can be simultaneously probed. Traditional solution heating and reaction monitoring technologies cannot achieve this aim.

In collaboration with investigators at the National Institute of Standards and Technology (Gaithersburg, MD), the Burden group helped develop a new method for rapidly heating a fluid, which allows a nanopore to measure the geometrical change of single molecules located near the pore opening. The new method involves locally heating a tiny volume of solution – a yoctolitre, or 10^{-24} litres – using a laser heat source that is focused by metallic nanoparticles. In the group's first work, the team attached gold nanoparticles (with diameters of 40 nanometres) to the top portion of a single nanopore. By irradiating the gold particles with a laser, 'surface plasmons' become excited. Surface plasmons are quantum phenomena – arising due to the oscillating charges of surface electrons. Exciting them causes the local temperature and viscosity of the solution to quickly change. Single target molecules located within this tiny volume can then be thermally driven into rare high-energy shapes, which are detectable when they are subsequently transported through the nanopore.

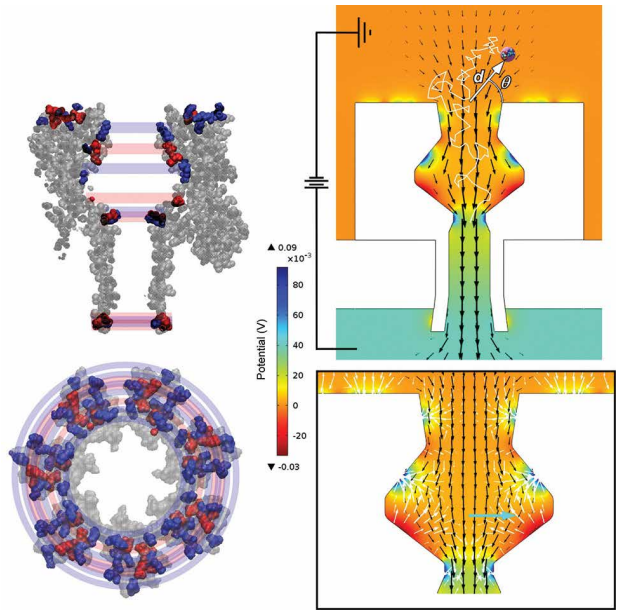
As a function of time and laser power, the group measured the consequent change in the conductivity of the surrounding solution. By measuring the conductivity change in the solution, the team was able to infer the extent of the temperature change and detect shape changes in single polymer molecules residing in the heated zone.

Their approach to measure optically induced temperature changes near nanopores has only been demonstrated with polyethylene glycol molecules thus far. However, this method has potential to be used for detecting conformational changes in proteins that undergo unusual and rapid folding processes and other complex changes, as well as studies aimed at unravelling the DNA double helix.

Simulating Membrane-Based Sensors

Some sensing measurements proposed for nanopores are experimentally complex. Furthermore, a vast number of different compounds might be detectable using nanopores. In efforts to narrow the immense investigative scope, computer simulations offer guidance to experimentalists who seek to discover and implement new applications. Simulations are able to predict current, force and temperature changes that occur inside nanopores, and to some extent, they can also predict similar changes in the surrounding solution. This enables researchers to predict the likelihood that a given molecular target will get drawn into the pore, where it can be characterised.

The voltage applied across a nanopore provides the driving force for entry of a target molecule, in what can be referred to as a molecular-capturing event. As a molecule in solution approaches the nanopore entrance, two kinds of forces are at work.



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Unidirectional 'drift producing forces' encourage targeted molecules to flow into the pore, like driftwood captured by a storm water drainpipe. However, at the nanometre scale, random directional forces, arising from frequent collisions with the target's molecular neighbours, become very significant. The forces arising from these impacts tend to push the target away from capture, competing against unidirectional drift through the channel. The relative size of the two opposing factors determines which type of motion dominates and also governs the likelihood of a capture event taking place. Interestingly, the relative balance of forces experienced by a target molecule depends on its distance from the nanopore and the strength of the applied voltage.

Drs Lisa and Daniel Burden have constructed a theoretical model to calculate the magnitude and direction of both the drift producing forces and the randomising forces for molecules as they approach and move through a nanopore. To do this, they combined a finite element analysis (FEA) method, in which a series of differential equations are used to calculate properties inside and outside the channel, with a Brownian motion thermal simulation. Using this approach, the team was able to plot force maps of unidirectional and randomising forces that a target molecule experiences as a function of location and applied voltage. By also looking at the erratic movement of the simulated target molecules, the team could calculate how likely a molecular capturing event would be for a given set of conditions.

Their results identified several critical limits that dictate the rates associated with molecular capture. These included the channel shape and size, the strength of the applied voltage, the salinity of the solution, and the size and charge of the molecule. The team's simulations demonstrated that under commonly used analysis conditions, random motion can disrupt directional flow, rendering a molecular capture event less probable. Significantly, their research ruled out certain types of complex sensor configurations, where the voltage required for high-probability capture is currently outside of realistic experimental tolerances. The simulations carried out by Drs Daniel and Lisa Burden offer a valuable resource for predicting the experimental conditions required to design functional sensing devices for molecular capturing events.

Future Directions for the Burden Group

The team now intends to collate their extensive experience with membrane-based sensors and work towards designing new controllable nanovalves. Their intention is to design tiny chemical valves that can be completely switched 'on' and 'off' on command, in a completely reversible and repeatable fashion, without the need for an externally applied voltage. Currently, the best ion channel candidates for valve operation only prohibit a small percentage of fluid flow, or are not reversible. So, the team is designing strategic chemical modifications to adapt channels for this application. Dr Daniel Burden states that the outcome will enable modified channels to operate 'much like a mechanical valve controls the flow of fluid in a pipe'. 'Just as today's macroscale manufacturing requires numerous types of mechanical valves to control the direction and type of fluid flow in complex machines, tomorrow's nanoscale manufacturing will require similar components that control molecular transport between tiny compartments,' he explains. These new nanovalves, with differing pore sizes and channel shapes, could be incorporated into small liquid-filled chambers, or even into the membranes of living cells to control what molecules enter and exit.

The Burden group's recent nanovalve work has shown that chemically modified channels can be stimulated to control bulk aqueous flow using reversible chemical interactions. Early work is being performed in both model lipid membranes and the more complex environment of biological cells. The team's results suggest that nanovalves embedded into cell membranes can control whether a cell lives or dies, by adding appropriate chemical triggers that open the valve to kill the cell, or close the valve to let it live. Furthermore, reversible molecular flow through the valve may be permitted over many 'on' and 'off' cycles.

This new type of nanoscale valve system also drives the need for new metrologies to gauge transport through the pore. Traditionally, researchers estimate the volume of molecular flow through its correlation with ionic current. However, this cannot account for the movement of neutrally charged compounds, chemical filtering effects induced by the channel's interior, or the potential cooperative effects of nanovalve aggregation. Thus, the team seeks to develop new optical approaches that will allow direct monitoring of materials moving through chemically modified nanopores. The new type of data promises to uncover relationships between chemical modification, channel shape and molecular size, which can then be used for optimising future nanovalve designs.

'The type and level of flow controlled by these nanovalves could create new horizons for many areas of science and engineering, such as enhanced chemotherapies, novel chemical sensors, new approaches to nanoscale manufacturing, and enable aqueous-based molecular electronic devices,' says Dr Daniel Burden. If the team achieves their concept of designing controllable nanovalves, the potential contribution that this technology would make is extensive.

Meet the researchers

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Dr Daniel Burden graduated with a PhD in Analytical Chemistry from Indiana University in 1997. Following a postdoctoral position in biophysics at the National Institute of Standards and Technology in Gaithersburg, MD, Dr Burden undertook a position at Wheaton College, where is he is currently Professor of Analytical Chemistry. Dr Burden's research includes methods to measure small molecules embedded into lipid membranes and observe their chemical and physical behaviours.

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Dr Lisa Burden graduated with a PhD in Biochemistry from Indiana University in 1996. She then undertook two postdoctoral positions at Indiana University and National Institutes of Health, USA before starting her current position as Visiting Associate Professor of Biology at Wheaton College in 2000. Dr Burden's primary research focus includes the study of toxin proteins produced by common bacteria and the chemical and biological interactions of these toxins with cellular lipid membranes.

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FUNDING

Camille and Henry Dreyfus Foundation
Research Corporation
Petroleum Research Fund
National Institute of Standards and Technology
National Science Foundation
Wheaton College Alumni Foundation

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Wheaton College

SMARTNANOTOX: DETERMINING THE TOXICITY OF NANOMATERIALS

Nanomaterials, owing to their unique material properties and activities, are popular for applications involving the detection and diagnosis of genetic and life-threatening illnesses, such as cancer. However, there is an academic and public concern over nanomaterial toxicity and their long-term adverse effects on the immune system. **The SmartNanoTox** team, comprising academic and industrial experts in *in-vivo* toxicity, was established to resolve the intricate mechanisms underlying nanotoxicity, and provide an efficient approach to predict the toxicity of nanomaterials.

The term nanomaterial describes a material, which is formed of individual units or particles that measure on the scale of 10^{-7}–10^{-9} metres in length. Each particle may be spherical, rod-shaped or fibrous with a relatively large surface area, depending on the fabrication methods and experimental conditions employed. At such dimensions, materials display unique optical, electronic and mechanical properties, often in remarkable contrast to their bulk counterparts. Although these materials are extensively used across the healthcare, environmental and automotive industries, questions about the potential effects that nanomaterials may have on human health, and how severe these effects may be, remain unanswered. This grey area of understanding has led to controversy over the safety of nanomaterials, creating a public perception of fear surrounding these critical functional materials.

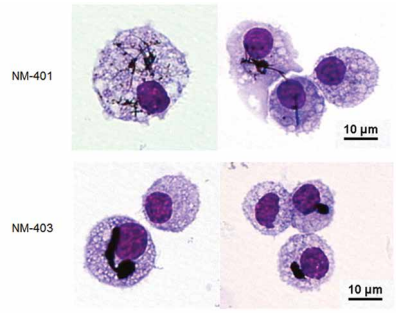
The specific mechanisms within living organisms that lead to adverse health effects after exposure to nanomaterials remain poorly understood. While some common industrial materials such as asbestos or quartz nanodust can cause a direct damage to animal or human lungs when inhaled, the effects of the many other nanomaterials can be indirect, delayed and complicated. Nanomaterials can accumulate within tissues and cause a chronic inflammation or distortion of the normal biochemical environment by producing reactive oxygen species or interacting with key biomolecules.

There is a current inability to accurately predict, based on their structure and activity, if a particular nanomaterial will display long-term toxicity effects in human cells and tissues.

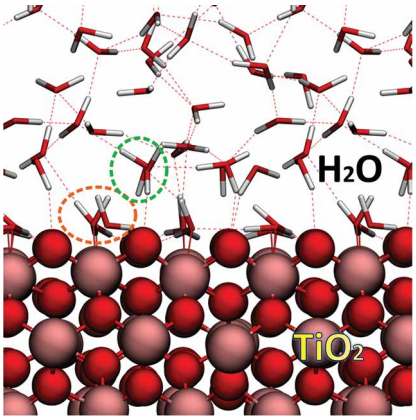
Nanomaterials can also enter a cell through its membrane receptors and cause adverse effects, such as the deregulation of cellular pathways. Deregulation and deformation of receptors and protein enzymes that participate in regulatory pathways can lead to the formation of neurodegenerative diseases, cancers, fibrosis and diabetes. Hence, a material that interferes with the regulation and function of these pathways in cells is also deemed as toxic. Although these networks have been extensively studied in numerous disease and DNA studies, there remains a distinct lack of understanding of the intrinsic mechanisms that lead to cell deregulation in the presence of nanomaterials.

SmartNanoTox: Smart Tools for Gauging Nano Hazards

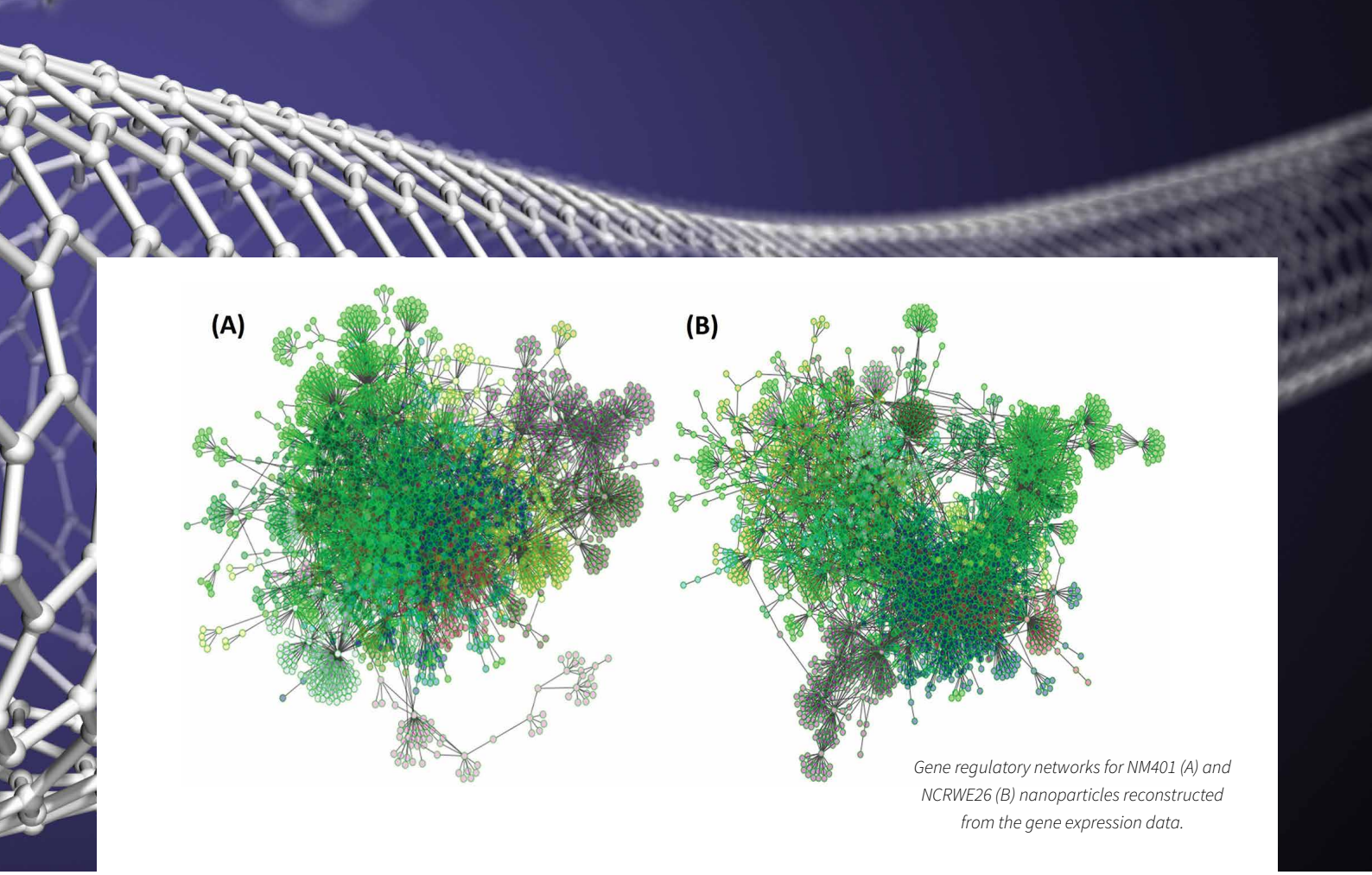
Dr Vladimir Lobaskin at the School of Physics, University College Dublin, Ireland, coordinates the SmartNanoTox project, which is funded by the European Union's Horizon 2020 research and innovation programme. The SmartNanoTox team is a collaboration between academics and industrial professionals with extensive experience in the field of *in-vivo* nanotoxicity, biophysics, materials science, and industrial



Lung alveolar macrophages containing carbon nanotubes (CNTs). Rats were exposed to nanotube aerosols (NM-401 and NM403).



Wetting of TiO_2 nanoparticles. Ab-initio molecular dynamics reveals details of water structure and reactions at TiO_2 nanosurface with atomistic resolution.



Gene regulatory networks for NM401 (A) and NCRWE26 (B) nanoparticles reconstructed from the gene expression data.

marketing. With members in Ireland, France, Germany, Slovenia, Denmark, Finland, Sweden and the UK, the team was recently established to further understand and resolve the underlying mechanisms of nanomaterial toxicity when inhaled. The primary aim of the project is to develop a mechanism-aware toxicity screening approach for nanomaterials.

Existing methods for predicting the toxicity of nanomaterials are based on measurements of toxicity performed on cell cultures *in-vitro* and on extrapolation of these data to *in-vivo* adverse outcomes. This extrapolation is often hard to justify because the exposure conditions (e.g. the dose and the state of the nanomaterial at the actual contact) and the activated adverse outcome pathways can differ drastically between the *in-vivo* and *in-vitro* setups. Moreover, without the mechanistic understanding of the toxicity, one has to rely on purely statistical correlations between the nanomaterial properties and the toxicity endpoints, where the mathematical model acts like a black box. The key to the progress in the development of predictive models lies in the detailed understanding of the response of the organism to nanomaterial exposure from the initial contact to the adverse outcome. The main hypothesis of the SmartNanoTox team is that this understanding can be achieved on the basis of system biology and new methods of characterisation and data generation in toxicology that have been developed in the recent years. This will finally lead to a new paradigm in the toxicology – a mechanism-aware nanomaterial toxicity screening.

Using a combination of *in-vivo, in-vitro* and *in-silico* approaches, the SmartNanoTox team will identify the mechanisms associated with the interactions between the nanomaterials and living organisms. At the systemic level, the team will use transcriptomics and proteomics data from *in-vivo* experiments, complemented by statistical modelling to identify the activated biological pathways and their corresponding molecular initiating and key events. At the molecular level, this will be achieved by analysing the state of the nanomaterial after the uptake, including their biomolecular corona and aggregation state, through both experiments and computational simulations. After this information has been gathered for a subset of nanomaterials, a sufficient set of data will be available, allowing for the identification of interactions leading to the activation of different toxicity pathways.

The SmartNanoTox team also intends to resolve all essential molecular interactions that can occur at the interfaces between biomolecules and nanomaterials, in a complete resolution of the structural deformation that a nanomaterial can cause when inhaled into the pulmonary system. The connection between different adverse outcome pathways and nanomaterial properties will be established through intelligent quantitative structure-activity relationships (QSARs), which will help to identify the properties of concern that should be avoided. The nanomaterials can then be grouped, according to their ability to participate in certain interactions and trigger specific adverse outcome pathways or disturb the normal function of the cells by interference in the key events of the pathways. Thus, an accurate scale of the *in-vivo* toxicity of nanomaterials can be defined and predicted without the need for extensive long-term testing.

The overall outcome of the SmartNanoTox project, if successful, will be the definitive ability to predict the *in-vivo* toxicity of a nanomaterial in an accurate and time and cost efficient manner, through the use of QSARs. As a consequence, the need for blanket toxicity testing and animal experiments will be reduced.

The SmartNanoTox team have made substantial progress in achieving the goals in their grant programme, several examples of which will now be detailed.

Panorama of recently opened super-resolution optical laboratory at the Jozef Stefan Institute, Slovenia.

Wetting TiO_2 nanoparticles

Titanium dioxide (TiO_2) is a common nanomaterial used in solar cells, self-cleaning materials and photocatalysis. The surface reactivity of TiO_2 nanoparticles can be tuned by varying the amount of water that is adsorbed to the surface of the material. Understanding the mechanisms that underly the modulation of this surface reactivity is crucial for unveiling the mechanisms that give rise to the toxicity of TiO_2 nanoparticles in the body.

In one particular study, the SmartNanoTox team reported computational simulations predicting the surface reactivity of TiO_2 nanoparticles. Using molecular dynamics modelling, the reaction of TiO_2 nanoparticles with differing concentrations of water can be simulated as a function of time. Simulations were run over a given time frame, and a comparison of initial and final structures were made to analyse the reactivity of the systems. Surface defects, such as missing and displaced atoms, are common in TiO_2. The team found that missing oxygen atoms promote water dissociation at the nanoparticle surface, and therefore increase reactivity. Furthermore, the concentration of water coverage that gives rise to the highest reactivity of water and the strongest interaction at the nanoparticle surface was identified for each naturally occurring crystal structure of TiO_2.

This work has demonstrated computational modelling to be a powerful tool for understanding the intricate mechanisms associated with nanoparticle reactivity.

Affinity of TiO_2 Nanosurfaces Towards Lipids

A large number of controversial cell viability tests has been reported for various TiO_2 nanomaterials. Focusing on the specific interaction between the nanomaterial and various plasma proteins and receptors, the Imperial College team has shown that a strong affinity exists between TiO_2 nanosurface and lipids.

With the affinity towards lipids being much stronger than that of silicon dioxide (SiO_2), the team discovered that at least certain morphological forms of TiO_2 nanoparticles can pull lipids out of membranes despite the free energy penalty arising from hydrophobic interaction and the curvature of the nanoparticles. This result has been proven using several physical methods, including fluorescence microspectroscopy and cross-correlation spectroscopy, super-resolution stimulated-emission depletion (STED) microscopy, and electron paramagnetic resonance spectroscopy (EPR). The team hope that understanding the mechanisms of the interaction between metal-oxide nanoparticles and lipids can predict the molecular initiating events in nanoparticle-exposed lungs, where various lipid structures are abundant. Their work reminds us that even an unspecific interaction between the nanoparticles and biologically relevant molecules can trigger adverse outcomes.

Device for in vitro exposure of lung cells to aerosolised nanomaterials under physiologically realistic conditions (VITROCELL CLOUD 6).

Modelling the Interface Between Cell Membranes and Nanomaterials

Nanomaterials can enter a cell in two different ways, either by active transportation through the receptors in the cell membrane, or passively by adhering to the cell membrane and causing it to bend and wrap around the foreign particle. Passive entry into the cell is only possible if the adhesion energy between particle and membrane is sufficient to compensate for the energy required to bend and deform the membrane.

Using molecular dynamic simulations, the SmartNanoTox team has derived a novel method to predict adhesion energies between soft lipid bilayers (which make up the cell membrane) and the solid surfaces of nanomaterials. Their approach involves fixing the two end points of the membrane bilayer being modelled in the simulation, and including a restraining force to allow realistic surface relaxation of the membrane, particularly at a curved interface. To increase the accuracy of the model, the mathematical descriptions of the interactions between the atoms were calibrated with experimental data. The final calculated adhesion energies could then be used to model the process of nanomaterials passively entering into a cell and predict if this process is energetically favourable.

Modelling the Nanomaterial Protein Corona

It is now well accepted that foreign surfaces are modified by the adsorption of biomolecules such as proteins or lipids in a biological environment, and that cellular responses to materials in a biological medium might reflect the adsorbed biomolecule layer, rather

Pathology laboratory and chief technician Sauli Savukoski. Finnish Institute of Occupational Health, Finland.

than the material itself. The composition of nanoparticle protein corona is flexible and is determined by many affinity constants and concentrations of the components of the biological fluids such as the blood plasma or the lung lining fluid.

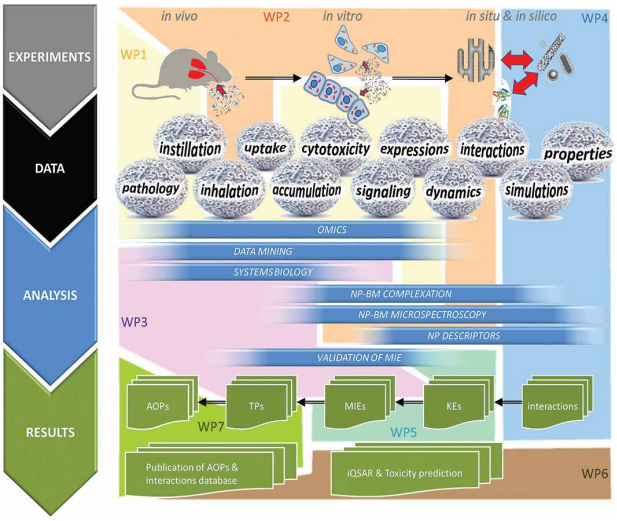
The SmartNanoTox team developed a framework for coarse-grained modelling of interfaces between nanomaterials and biological fluids and membranes. Their model includes united-atom presentations of membrane lipids and proteins, which are based on all-atom structures of the corresponding molecules and are parameterised using experimental data or atomistic simulation results. The nanoparticles are modelled by two-layer objects, where the nanoparticle shell reflects the interaction between the material and the biomolecule in the corresponding fluid, while the core interacts with the biomolecule through van der Waals forces.

The proposed methodology can be used to predict the adsorption energies for dozens of common human blood plasma proteins on nanoparticles of different sizes, as well as the preferred orientation of the molecules upon adsorption. With these energies, scientists will be able to rank the proteins by their binding affinity to nanomaterials, and predict the composition of the nanoparticle protein corona for the corresponding material. Finally, these data will be used to construct a bio-nano interactions database and QSARs for the selected adverse outcome pathways.

Inhibiting the Dynamics of Cell Fate Decisions

Changing the dynamics of protein activation in cellular networked pathways, such as the pathway between RTK/RAS/RAF/MEK/MAPK protein kinases, can lead to protein mutation and disease formation.

On this topic, the SmartNanoTox team reported a review of methods that regulate the dynamics of the MPK kinase, which is associated with cell fate decisions and drug resistance. In particular, the review highlighted that physiological factors can control and modulate cell decisions. Mechanisms within the protein networks can be probed using new techniques such as biosensors and microfluidics, while biochemical responses and their associated timescales under applied external stimulus can also be measured. Mathematical models can also shed light on the expected time scales for each mechanism, thus further resolving the intricate chemical mechanisms associated with cellular protein networks.



Outline of the project concept. Abbreviations used: WP – work package, BM – biomolecule, NP – nanoparticle, AOP – adverse outcome pathway.

Hyperactivation of the RAS/MAPK pathway is reported to be the cause for over 30% of human cancers. Inhibitor drugs act to deactivate such hyperactivated pathways, but a serious problem associated with their use is drug resistance. The origin of this resistance is the formation of chemical bonds between two protein kinase complexes, and the SmartNanoTox team has shown that kinase dimerisation is thermodynamically favourable, once an inhibitor molecule is bound to a kinase protein. It is therefore the binding affinity of the inhibitor for the kinase protein that will dictate if drug resistance to pathway inhibitors is thermodynamically favourable.

Summary

- The measurement of the long-term effects of nanomaterial toxicity on human health is expensive and time consuming, requiring extensive animal testing and verification experiments.
- The SmartNanoTox team, coordinated by Dr Lobaskin at University College Dublin, is funded by a 2020 Horizon European grant to resolve the underlying mechanisms and biochemical pathways that regulate *in-vivo* toxicity of nanomaterials.
- The main focus of the SmartNanoTox team is to provide a mechanism-aware method to predict nanomaterial toxicity based on the generation of quantitative structure-activity relationships between the nanomaterial properties and their ability to trigger adverse outcome pathways.

Meet the researchers

Professor Vladimir Lobaskin

Dr Vladimir Lobaskin is Head of the SmartNanoTox team and is an Associate Professor in the School of Physics at the University College Dublin, Ireland. Throughout his academic research career, Dr Lobaskin has made significant contributions to the field of theory and modelling of nanostructured biosystems, including the development of computational approaches and software (MOLSIM and ESPResSo) for modelling soft-matter systems.

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 686098.

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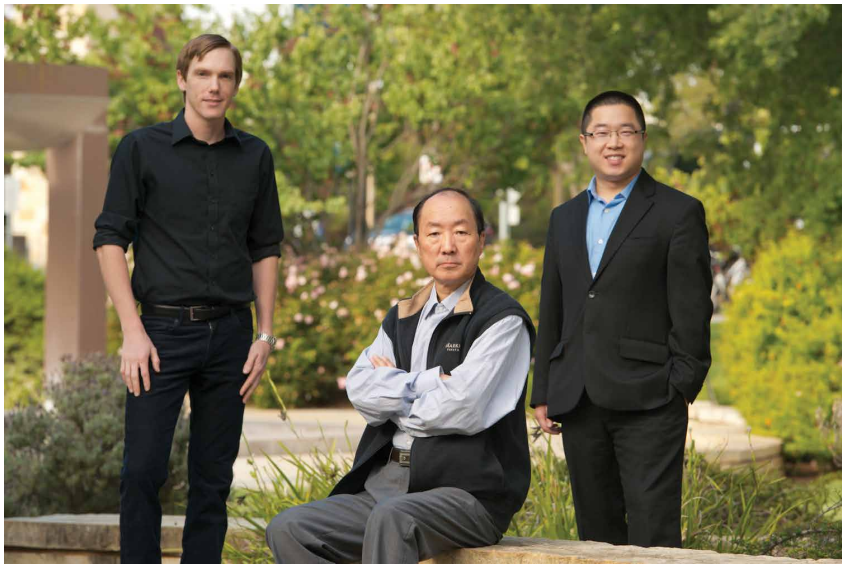
THE SCIENTIFIC AND MATHEMATICAL WORLD OF TEXTILES

Textiles, including rope and yarn, are often thought of as functional and convenient materials for us to dress in, suspend swings from (in our more youthful days), or to safely secure items during transport. However, behind such critical applications is a complex understanding of mathematical and scientific mechanisms that give rise to unique material properties. It is within this scientific field that **Professor Ning Pan** at UC Davis has established his academic career.



The textile industry is one of the oldest and most traditional known to humankind. Indeed, the conversion of natural fibres into textile commercial products can be predated to the Paleolithic era, over 3.3 million years ago. With current global production of cotton-based products alone exceeding millions of tonnes every year, the socioeconomic importance of the textiles industry is evident and irrefutable.

Natural fibres, such as cotton, or synthetic fibres, such as polyester, are harvested or manufactured, and then twisted and combined into a substructure – referred to as a yarn. The manner of the combination can be changed and varied to form yarns of differing radial cross sections, until they form strands with a defined geometry – a helical fibre path is the form a strand can adopt. Strands can either be used to make fabrics for clothing or furnishing products, or can be further combined and manipulated into specific geometries to form rope.

Professor Pan at the University of California, Davis, has dedicated his academic career to investigating the material properties of fibrous textiles and modelling the structures to optimise their use in clothing, and in other applications throughout the textiles industry. 'From a dynamic perspective, the human-body-environment system is highly complex, and unfortunately is still poorly understood,' Professor Pan states. 'It remains elusive how exactly a cloth can keep us warm and comfortable.' With such seemingly basic concepts remaining unexplained, he believes that 'many novel scientific discoveries can thus be achieved in this area'.

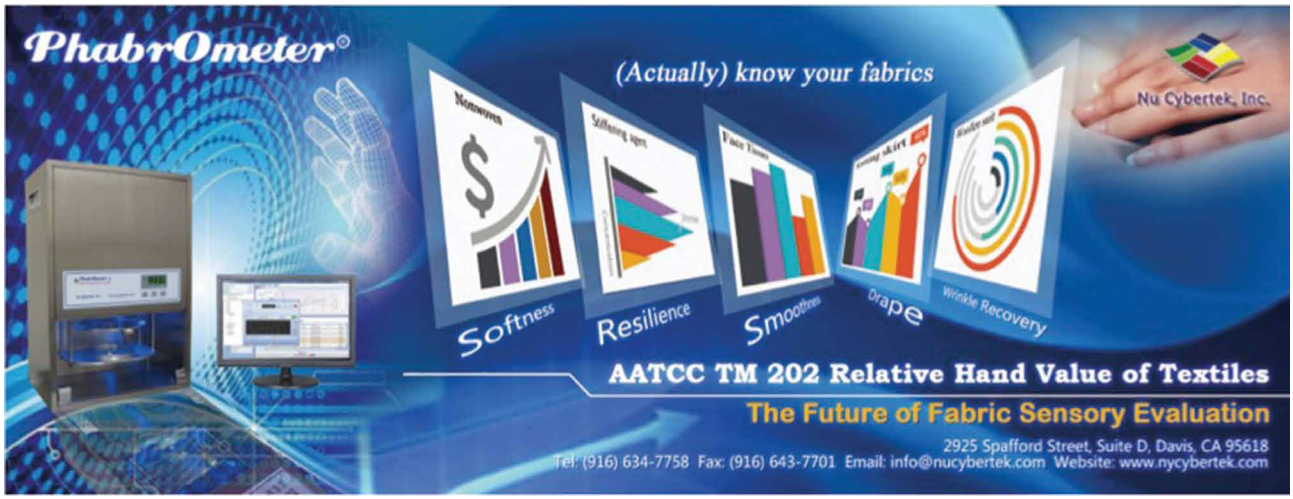
The Mechanical Strength of Twisted and Woven Textiles

The importance of resolving the mechanisms underlying the mechanical strength of rope and yarn has been historically recognised 'as far back as Galileo', as highlighted in a review written by Professor Pan. When combined into a strand and then a rope, factors such as the interaction between fibre segments, geometry of strand combinations and distribution of strain across a local area of the material, must be considered for accurately predicting mechanical properties.

To estimate the elastic properties of yarn or rope, the stress-strain relationships as a function of Cartesian displacement in the longitudinal and transverse directions of a yarn must be calculated. Professor Pan has made significant contributions to the derivation of computational models to accurately describe the tensile strength and elastic properties of yarns and ropes, alongside conducting experimental work to validate and improve these models.

Using general approaches to predict the stress strain relationships of yarns is not sufficient for an accurate prediction of elastic properties. Because of this, Professor Pan's team investigated the influence of factors such as fibre tension, lateral compression and hybrid effects on the mechanical

‘How cloth interacts with our body and the outside environment critically determines our physical, physiological and even psychological wellbeing. Our research efforts focus on understanding the complexities in this system so as to improve the performance of the cloth and to better serve the increasing demand from consumers.’



properties of fibres, when more than one fibre types are combined. They realised that the intrinsic tensile strength of smaller fibres is greater than that for longer fibres, a consideration which had been neglected in previous models. Finally, Professor Pan’s team explored the effects of steric hindrance in fibres, where new contacts made between fibres are affected by neighbouring interactions in other regions of the material. To combine all of these factors together, Professor Pan has developed theoretical models, to yield a comprehensive and accurate approach to predicting their complex mechanical properties.

A woven textile fabric is also formed from the combination of yarns, but instead of forming a strong, high-density mass of strands, woven fabric yarns are cross-linked in various patterns though interweaving. The locations of the interfaces between interwoven yarns are referred to as the interlacing points. The interactions between yarns at the interlacing points significantly enhance a fabric’s strength.

By reporting the first full computational and experimental study into the origin of tensile strength in woven fabrics, Professor Pan was able to show the exact mechanisms that cause tension to build up at the interlacing points, and how tension is then acquired throughout the fabric. Based on several factors, Professor Pan was able to calculate the tension and displacement in a woven material when fibres are fractured or pulled out of the interwoven pattern.

Professor Pan team’s theoretical models have provided a way to predict the optimum material properties for a given application, thus reducing the need for experiments when designing and creating new textiles.

A Mathematical Description of Uncomfortable Clothing

The formation of rashes and blisters from uncomfortable clothing is often caused by high stress and friction between fabric and skin. Factors such as the fabric properties, fabric-skin gap and fabric-skin interactions all dictate the extent of stress at this interface.

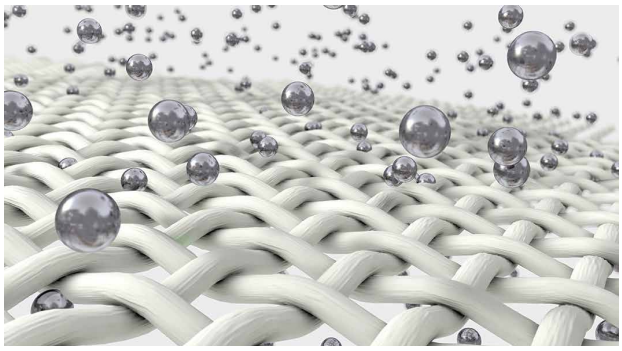
Professor Pan was the first academic to quantitatively show that poor garment design results in adverse skin reactions. His team’s simulation used an explicit finite element (ELE) model of a forearm in contact with a garment layer. This model, created by Professor Pan and his colleagues, considered a 3D cylindrical forearm shape with an inner bone core, surrounded by a layer of muscle, and encased in a layer of skin. To calculate the stress formation and friction coefficients between the garment and skin, the ELE model adopts a numerical approach, using analytical differential equations to represent a layer of material by its elastic properties, instead of explicitly modelling the microscopic atomic structure.

Professor Pan and his team designed the model of the forearm to include a gap between garment and skin on the arm. With rotation at a defined angle with an associated speed (which represents a realistic arm rotation), the sleeve of the garment is allowed to drop freely under gravity. The sleeve then strikes the skin and the stress response between the layers can be calculated. This research explicitly demonstrates that poor garment design can directly lead to skin irritation and discomfort following arm rotation.

Assessment of Textile Sensory Properties

For many fibrous consumer products (textiles, paper and leather etc.), human sensory perceptions to products (hand, touch, appearance) are critical for consumers to judge the quality and make a purchase decision. Yet, these properties are very subjective and hard to measure reliably.

Professor Pan has developed an instrument, the PhabrOmeter®, to assess the sensory properties (tactile and visual attributes) of textile products. The instrument provides critical yet currently unattainable sensory quality information with potential impact on multiple industries including textile, nonwoven, paper and leather, and skincare products. It has become a designated standard machine by the US America Association of Textile Chemists and Colorists



(AATCC) for fabric hand evaluation, and has been adopted by several dozens of clients worldwide, many being Fortune 500 companies.

Sweating for Infrared Camouflage!

Suppressing the heat signature caused by temperature fluxes of the human body is the principle behind Infrared (IR) camouflage. To date, scientists have come up with a number of approaches to achieve IR camouflage, including dispersing aerosol particles in the atmosphere to scatter IR radiation, coating materials with a substance that is less emissive to IR radiation, and using phase change materials (PCMs). PCMs change the absorption and emission of latent heat, thus modulating their surface temperature and IR emissivity.

Professor Pan recognised that the human body has its own natural PCM, which regulates the temperature of the body – sweat. Sweating is the body's natural cooling mechanism and is effective due to the high latent heat of vaporisation of water. Professor Pan and his colleagues designed a textile prototype, which facilitates sweat transport and controls the surface temperature of skin. The prototype design involved four layers of material. The inner most layer, layer 1, absorbs sweat from the surface of the skin into layer 2. Layer 2 then encourages the skin to sweat by supplying latent heat. Layer 3 possesses a high porosity to retain sweat, and between layer 3 and layer 4, sweat evaporation takes place. A mathematical model describing the transport of the sweat through the 4 layers was used to optimise layer thickness and porosity at a given temperature and humidity to achieve the most efficient IR camouflage.

Clothing that can achieve IR camouflage can be used in applications to control skin temperature in extreme environments and also within the defence and military sectors to conceal personnel.

Thermal Conductivity of Fibrous Textiles

Thermal conductivity is described as the transport of heat throughout a material. The long-range elastic vibrations of a material lattice dictate its ability to transport heat. Lattice vibrations are quantum mechanical wave-particles called phonons, and the ability of a material to transport these phonons can vary drastically depending on the material properties. Textile materials possess short-range order with non-homogeneous fibre orientation and cross-linking interactions, which result in inefficient thermal transport and short-range phonon transport paths.

Professor Pan reported the first analytical model that could accurately predict the bulk thermal conductivity of fibrous materials, which could account for material structure effects. His team used a random generation-growth algorithm to generate different structural orders of the fibres, including a differing extent of fibre orientation, cross-linking interactions and porosity. Once the team had generated a subset of structures, they used a lattice Boltzmann equation to solve known energy transport equations as a function of temperature, which gives a thermal conductivity value for fibrous textile structures. A complex multi-conjugate heat transfer method allowed the team to determine the average thermal conductivity through an inhomogeneous material. The team's model was confirmed by experimental measurements to accurately predict thermal conductivity as a function of fibre size, fibre orientation and material porosity.

Modelling Liquid Transport in Textiles

The scientific understanding of the properties and liquid transport in wet textiles is crucial in applications such as lubrication, clothing and composite manufacturing. Gaining an understanding of the capillary action involved in liquid transport and flow is an active field of materials research.

Professor Pan and his colleagues created computational simulations describing the flow and transport of liquid in a textile material formed of fibres. These types of simulation – known as Monte Carlo simulations – are often used to study the macroscopic distribution of variable features in a structure, such as the orientation of fibres. They constructed a large model, consisting of 36 cubic cells, each filled with gas, liquid or a fibrous mass with constant initial orientation. The total energy of the system and the energy associated with a change in the orientation of a single fibre are predetermined constants. The simulations can be run for a period of time at a given temperature, thus allowing the team to predict the equilibrium configuration of fibre orientation and distribution throughout the simulated structure. The simulations allow for the movement of liquid and gas through the fibre mass, resulting in a flow process through the material being modelled.

The probability for change in fibre orientation is dictated by the Boltzmann distribution according to the available thermal energy. Professor Pan has demonstrated that simulations using his model are able to accurately predict the dynamics and structural changes in fibres with liquid transport.

Future Directions

So what lies ahead for Professor Pan and his team? Currently, they are developing a new systematic framework approach to support scientific researchers. 'Such a systematic framework has been lacking so far and is desperately desired by both scientific community and industry,' Professor Pan explains. 'A rigorous theoretical framework can guide the new researches along the right direction and with a clear and comprehensive perspective.'

Meet the researcher

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Professor Ning Pan was awarded his PhD in Textile Engineering from Dong Hua University in Shanghai, after which he took a postdoctoral researcher position at Massachusetts Institute of Technology, USA. He then became an Assistant Professor of Fiber & Polymer Science at UC Davis, California, USA, before being promoted to his current position as Professor of Fiber & Polymer Science in 1999. Professor Pan is the recipient of many internationally recognised honours, including Fellow status from the American Physical Society and the Nano 50 award from NASA Tech Briefs. Parallel to his research and expansive publication history, Professor Pan is a board member for several international journals, and has also been awarded multiple patents, including patents for the invention of the PhabrOmeter. The PhabrOmeter allows the measurement of sensory quality information of textile products and has made significant contributions to the textile and skincare product industries. Professor Pan has established an extensive academic career, with research focuses including computational modelling of soft fibrous materials, synthesis and characterisation of carbon nanotubes for super capacitors and batteries, human-cloth microclimates and the performance evaluation of consumer products.

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HYPERSONIC LASER TAGGING: A NEW WAY OF UNDERSTANDING FLUID MECHANICS

Fluid mechanics is the study of the flows within liquids, gases and plasmas, and the forces that act upon them. Applications involving fluid mechanics are vast, ranging from chemical engineering to astrophysics, and so an accurate understanding is essential for future developments. **Professor Richard Miles** at Texas A&M University is an esteemed contributor to this field, and his team's latest breakthrough involves a pioneering way of measuring the velocities of high-speed fluids.

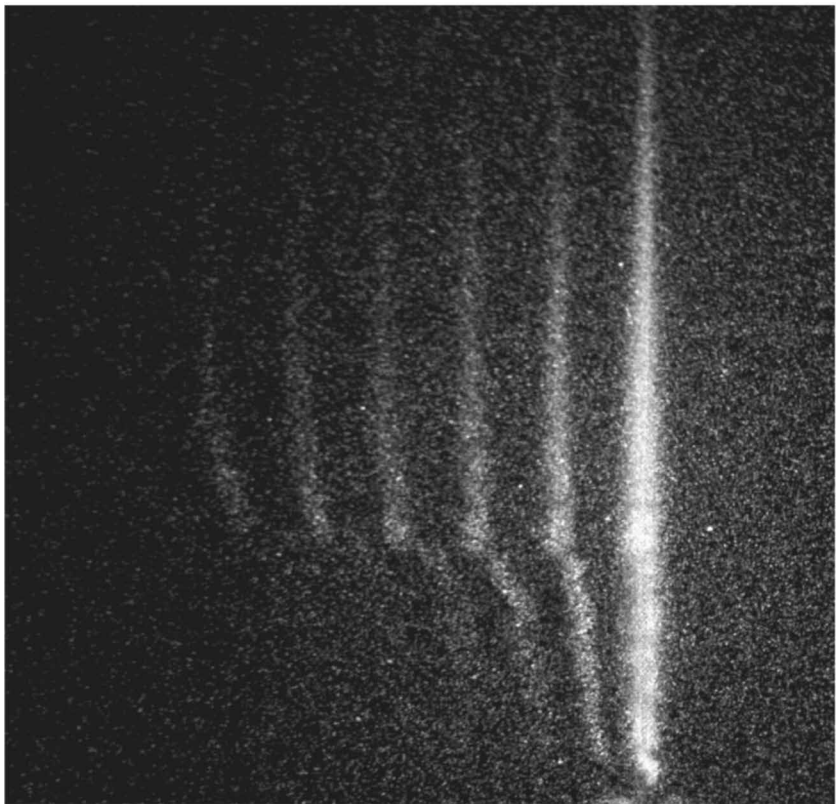
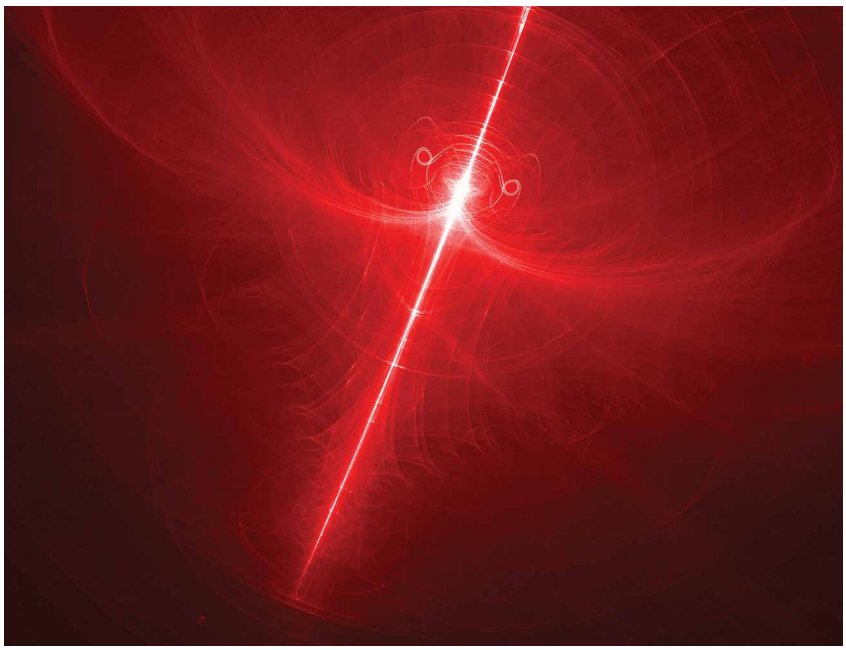


Figure 1: A single FLEET line tagged across a Mach 3 boundary layer in a nitrogen flow sequentially imaged at three microsecond intervals. Flow is from right to left. Image was taken at the Arnold Engineering Development Complex, White Oak, Maryland

Like a gust of wind or an ocean current, most flows within fluids are invisible to the naked eye, and as such, techniques have been developed to visualise these complex and dynamic patterns. The beginnings of a scientific approach to flow visualisation can be traced back to experiments performed by Leonardo da Vinci. It is said that he would float grass seeds in moving water and sketch their resulting trajectories. After repeated sketches, information about the flow of the fluid could be determined, and by measuring the position of the seeds over time, the velocity of the flow could be estimated in a process known as 'velocimetry'. Whilst modern velocimetry methods have become much more accurate and intricate, many still use this basic principle, where the flow is 'seeded' with particles that can subsequently be observed and recorded.

However, with all techniques that seed the flow, a degree of inaccuracy is incurred. For example, if using smoke to visualise the flow within air, the assumption is made that the smoke particles faithfully follow the fluid flow pattern. In reality, given that they are a different density and consistency, this is unlikely to be the case. Even particles with densities matching that of the fluid may have other physical differences that will cause some disruption to the flow.

An alternative to intrusive seeding techniques is the innovative method of velocimetry known as 'molecular tagging'. Simply put, this technique uses a laser to chemically or electronically alter some molecules within the flow as they pass through its beam. The molecules that are hit by the laser can then be visually distinguished and are said to be 'tagged', but they keep the same physical behaviour as the rest of the fluid. Conventionally, the laser is positioned perpendicular to the flow of the fluid so that a line of tagged molecules is produced from the beam across the whole flow. This then gives a representative sample of the flow, and as this line of tagged molecules is transported by the movement of the fluid, images at two intervals of time are produced to determine how the line of tagged molecules is being displaced or deformed.



What is FLEET?

Femtosecond Laser Electronic Excitation Tagging (FLEET) is a special velocimetry technique developed by Professor Richard Miles and his research team at Princeton University. Central to this effort was the work of Matthew Edwards, Princeton class of 2012, Dr James Michael (now at Iowa State University), and Dr Arthur Dogariu.

Professor Miles has recently accepted the position of TEES Distinguished Professor at Texas A&M University (TAMU) and plans to implement FLEET at TAMU in their high speed aerodynamic facilities. Essentially, the technique takes advantage of unique properties of recombining nitrogen molecules by first dissociating them with a titanium-sapphire laser pulse with tens to hundred of femtosecond duration. This short pulse avoids the formation of bright sparks and enables the writing of lines and patterns of dissociated species into the flow. After dissociation, the nitrogen atoms recombine, forming nitrogen molecules in a high-energy state that emits fluorescent red and infrared light for tens of microseconds (first positive emission).

This extended fluorescence time allows the flow to move far enough for the displacement to be imaged with a fast-shuttered camera, and the displacement divided by the time delay gives the flow velocity. The technique is specifically attuned to nitrogen – the most abundant molecule in air – and so the aerodynamic flows can be followed in real time, without disrupting the flow with foreign gases or obstructive particles. Due to FLEET being non-intrusive on the flow of the fluid and providing an instantaneous profile of the flow, it has the potential to yield unprecedented insights into high-speed fluid mechanics. The ability of FLEET to write patterns into the flow, such as crosses and rectangles, enables the measurement of vorticity, shear stress and other dynamic flow properties.

FLEET is aptly named, because it has the capacity to measure fluid velocity at incredibly high flow speeds. If the camera has a multiple time-gated shutter, the motion of a single line can be followed in real time. For example, Fig. 1 shows sequential 3 microsecond-delayed images of a single line tagged across the boundary layer in a Mach 3 nitrogen flow (flow is from right to left). If a flow is more than five times the speed of sound, it is generally described as 'hypersonic', and a non-intrusive way to directly measure the velocity and other properties of these rapid flows has remained elusive for some time. FLEET is able to accurately measure flows from subsonic to hypersonic speed because the laser beam is non-intrusive and pulses in the femtosecond range (quadrillionths of a second). There are other techniques available that can indirectly measure the velocity over this range of speeds, but unlike FLEET, they require two separate lasers, or they require a foreign gas or particles to be added to the flow. More conventional methods using probes disrupt the flow.

Another advantage of using FLEET is that the nitrogen molecules emit visible red light when they are excited by the laser, so there is no need for specialised equipment to detect the tagged molecules in the ultraviolet or infrared spectrum – a standard camera with a time gated intensifier is sufficient. Not only this, but the technique has been shown to be functional at a wide range of pressures and temperatures, and has the ability to measure thousands of samples a second.

The Development Process

In the 1980s, Princeton University developed the world's first system able to perform the molecular tagging of air. This method was known as Raman Excitation plus Laser Induced Electronic Fluoresce (RELIEF), and worked by tagging the molecular oxygen that is present in air. It proved to be an extremely useful method for measuring the velocities of turbulent flows, and applications of RELIEF made possible the measurement of high pressure, supersonic jets. However, the setup was impractically complicated, by requiring three overlapping laser beams and an ultraviolet sensitive camera.

There was an obvious need for a more practical design, and so Professor Miles and his team put together a transportable FLEET setup so it could be moved to relevant high-speed facilities and be able to track the motion of air and nitrogen in real time. He and his team demonstrated this transportable setup in the 'nitrogen hypervelocity wind tunnel', Tunnel 9, at the Arnold Engineering Development Complex (AEDC), at wind speeds of up to 14 times the speed of sound. This work was conducted in collaboration with Dr Eric Marineau and Mr Michael Smith at AEDC and was implemented by Dr Laura Dogariu and Dr Arthur Dogariu in association with Plasma TEC, Inc and Speckodyne, Inc., through a Phase II SBIR grant.

The velocities measured by FLEET were in excellent agreement with the predicted results from standard wind tunnel gauges. Fig. 2 shows the time history of the FLEET measurements taken at a 1 kHz rate along with the predicted velocity of the Mach 14 flow, including the start up and shut down transients. Note that the flow velocity increases during the three-second constant Mach number run due to the increase in temperature of the nitrogen in the wind tunnel settling chamber. This is the first time a direct measurement of the flow velocity has been achieved in this facility.

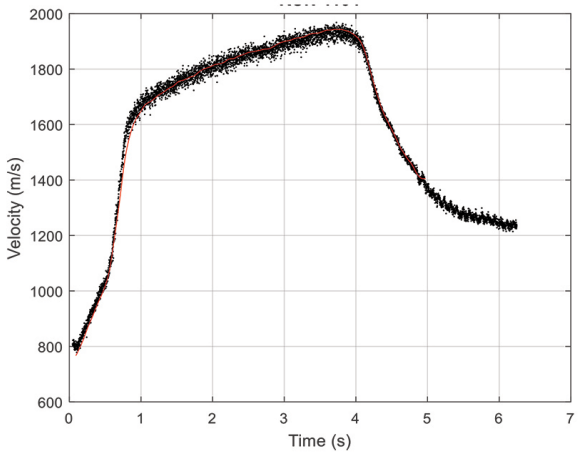


Figure 2: Nitrogen flow velocity versus time in the AEDC Tunnel 9 operating at Mach 14. Measured points are black and the predicted velocity profile is shown in red.

Breaking New Ground

For the first time, FLEET has also been used to measure three components of a flow's velocity and acceleration in collaboration with Dr Paul Danehy at NASA Langley Research Center. The measurements were conducted in a jet of pure nitrogen that was injected into air at atmospheric pressure. The femtosecond laser that FLEET uses can be focussed down to a fine point, so that only a small volume is measured in the flow. Because FLEET creates excited points that have long fluorescence lifetimes, they can be measured at several different instances, and by using a cleverly positioned mirror setup, stereoscopic images of the moving FLEET points can be projected onto the camera simultaneously. This allows for three components of the velocity to be measured at once, providing a highly accurate measurement of the three-dimensional flow velocity as well as the acceleration of the flow.

Not only can FLEET determine flow velocity with an excellent degree of precision, but by using it in combination with a spectrometer, it has recently been adapted to measure the temperature distribution within the flow too. Spectroscopy is the study of the interaction between matter and light. When nitrogen molecules are excited they also emit blue light that lasts for only a few tens of nanoseconds. The spectrum of this blue 'second positive emission' gives an immediate measure of the temperature within the flow. These temperature profiles are determined within a reasonable uncertainty of 10%, and Professor Miles' team has performed these measurements at conditions ranging from room temperature to nearly 400°C.

It is predicted that this method of measurement will remain accurate at temperatures far exceeding 1500°C, with velocity measurements being conducted simultaneously without any interference. Very few methods and techniques can simultaneously measure temperature and velocity, and dual measurements such as these become extremely difficult under the conditions of hypersonic speeds and or high-pressure environments. FLEET's ability to do this has far-reaching applications in industry and any field of fluid mechanics.

A Future in Industry

Most measurement techniques deduce the velocity of a fluid's flow from indirect methods. Commonly, a so-called 'pitot tube' is used to indirectly measure velocity by directly recording changes in pressure. Another method employs a 'hot-wire anemometer', which is a simple metal wire device that is heated to above room temperature. As the fluid flows past, it cools the wire. Electrical resistance in most metals is related to temperature, and so, depending on the degree of cooling that occurs, a relationship can be established between the resistance of the wire and the flow speed. These techniques have been applied to a wide range of flows with much success; however, their shortcomings are that they do not directly measure molecular motion, and can also be disruptive to the flow. Also, the approaches of pitot tubes and hot wires have limited adaptability to industry because of the size of the probes cannot be scaled while maintaining high accuracy.

Although there are a variety of different seeding techniques used for measuring velocity in fluid mechanics, adapting these techniques widely to large-scale industrial uses still has not occurred. This is in part due to the requirement of the flow to be seeded with particles or potentially toxic gases, and so most facilities are unwilling to upgrade their current setup to accommodate these seeding velocimetry techniques. Therefore, these 'unseeded' techniques developed by Professor Miles and implemented by FLEET have great potential in both small and large scale industrial applications.

The future of FLEET is looking bright – from subsonic to hypersonic flow velocities, under high-pressure or high-temperature conditions, FLEET's strength is in its simple, elegant design. The revolutionary approach of using one commercially available laser and one camera to directly and non-intrusively measure the velocities of fluid flows in air has the potential to make waves within the industry. Not only this, but FLEET's aptitude for adaptability is one of its most exciting advantages. By adding a spectrometer, Professor Miles and his team have shown that the temperature of the flow can be determined; however, there is also the possibility to calculate the density of the flow by measuring how much the laser beam is scattered by nitrogen molecules in the air (also known as 'Rayleigh scattering'). Additionally, the FLEET setup could easily be modified to accommodate several cameras, which would provide a stereoscopic, 3D image of the flow, and by using a camera with a rapid shutter speed, taking multiple images could generate a model of how the flow distorts over time.

Meet the researcher

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Professor Richard Miles received his BS, MS, and PhD in Electrical Engineering from Stanford University. His PhD was conducted under Prof Stephen E. Harris and addressed third harmonic generation of coherent light. While at Stanford, he became a Fannie and John Hertz Fellow. He joined the Mechanical and Aerospace Engineering faculty at Princeton University in 1972, and later served as Chairman of Engineering Physics there for over 15 years. He was named Robert Porter Patterson Professor in 2011 and became Emeritus in 2013. Professor Miles joined the Departments of Aerospace Engineering and Mechanical Engineering at Texas A&M University (TAMU) as TEES Distinguished Research Professor in February 2017. While primarily in Texas, he continues to oversee his Princeton research activities as a Senior Scholar. His research focuses on the use of lasers, electron beams, microwaves and magnetic devices to observe, control, accelerate, extract power and precondition gas flows for supersonic and hypersonic fluid dynamics, combustion, propulsion and homeland defence applications. His research group is widely recognised for inventing new linear and nonlinear optical diagnostics, developing a new understanding of plasma aerodynamic interactions and exploring new concepts for hypersonic ground test facilities.

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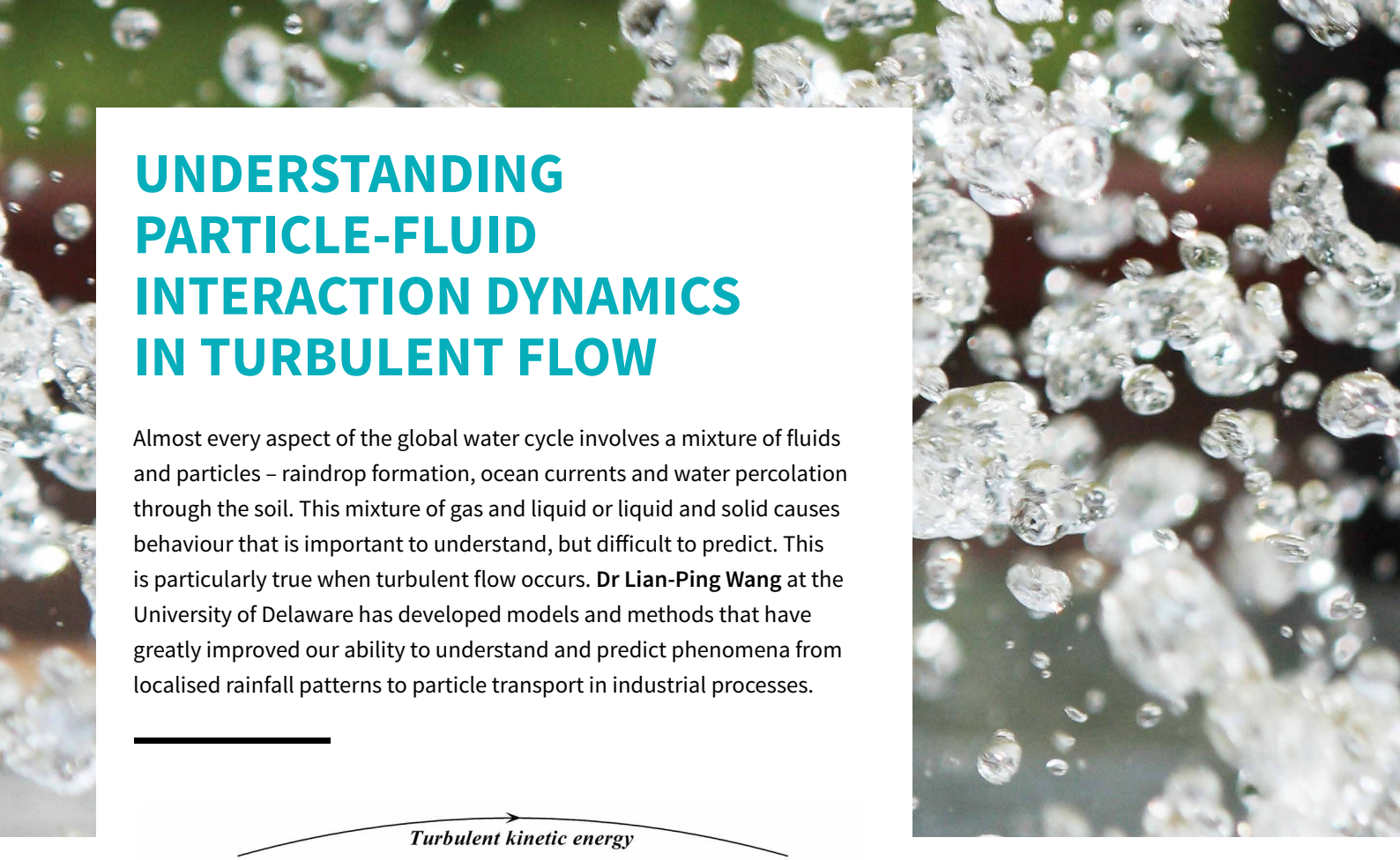
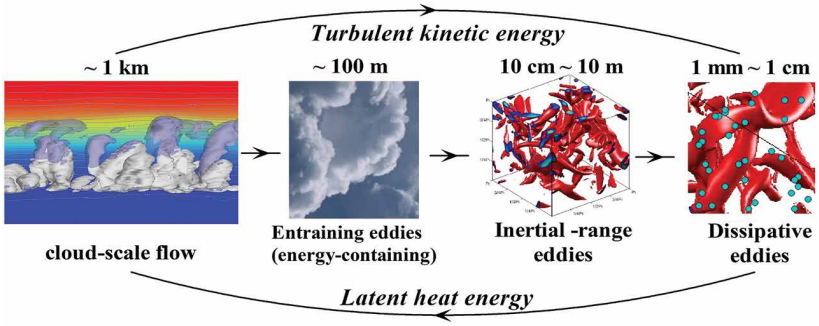
FUNDING

US Air Force Office of Scientific Research, Hypersonics Program under Dr Ivett Leyva
US Army Research Office, Fluid Dynamics Program under Dr Matthew Munson
US Air Force Arnold Engineering Research Complex
MetroLaser, Inc.
Plasma Tec., Inc.



UNDERSTANDING PARTICLE-FLUID INTERACTION DYNAMICS IN TURBULENT FLOW

Almost every aspect of the global water cycle involves a mixture of fluids and particles – raindrop formation, ocean currents and water percolation through the soil. This mixture of gas and liquid or liquid and solid causes behaviour that is important to understand, but difficult to predict. This is particularly true when turbulent flow occurs. **Dr Lian-Ping Wang** at the University of Delaware has developed models and methods that have greatly improved our ability to understand and predict phenomena from localised rainfall patterns to particle transport in industrial processes.



Multiphase fluid flow occurs when flows contain multiple phases of matter, such as raindrops in air, and river water mixed with sediment. Many environmental processes involve multiphase flow, as do many industrial activities. Multiphase flow, particularly when it is turbulent and complex, is difficult to predict and can present unexpected phenomena. Many questions exist about how these phenomena occur or how processes may vary under different conditions.

Creating rigorous simulations of these multiphase systems is often the best way to try to understand them. Almost all work on understanding fluid dynamics starts with the Navier-Stokes equations, which link the local movement, pressure and temperature of a fluid. An important parameter in a flow system is the 'Reynolds number', which is calculated from the domain length scale, density, velocity and viscosity of a fluid. Low values of the Reynolds number are associated with smooth 'laminar' flow, while high numbers imply turbulent flow with vortices of different shapes and length scales. This multiphase turbulent flow is, not surprisingly, harder to simulate. However, it is also much more commonly found in real-world fluid flow. The chaotic, seemingly random behaviour of turbulence cannot be solved analytically with the Navier-Stokes equations, and so must be modelled or solved using other approaches. Numerical simulations are the commonly used approaches that split the fluid up into small parcels or cells, and calculate the movement, pressure and other factors within each cell as a result of the influence of the surrounding cells. A particularly powerful numerical approach is known as the direct numerical simulation (DNS), where the Navier-Stokes equations are integrated directly without modelling. DNS can be viewed as a numerical experiment of a turbulent flow system.

DNS requires a lot of computing power and also great expertise, in order to mathematically represent the real physical processes taking place in the best possible way. Dr Lian-Ping Wang of the University of Delaware is an expert in this field, and his team has been tackling the challenges of turbulent multiphase flow using DNS. 'My work is fundamental in nature, but with a very broad application for industrial and environmental processes,' says Dr Wang.

Simulating Real-World Processes

Weather prediction relies on simulation models that predict the movement and behaviour of parcels of air at a global scale. Because of the enormous computational requirements, these parcels of air need to be quite large to avoid having too many of them for the simulation to cope with. As a result, it is difficult for global models to simulate weather conditions at a small scale (e.g. less than a kilometre). Having this information would be very important, particularly for forecasting extreme weather effects caused by climate change. This could help us to better prepare for landslides, flooding or damage to buildings and crops at specific locations.

One process of particular interest to Dr Wang and his team is the formation of raindrops from cloud droplets. This is influenced by many factors, including air humidity, temperature and pressure, but it is also strongly affected

‘My work is fundamental in nature, but with a very broad application for industrial and environmental processes, such as weather and climate, combustion, particle technology, and contaminant transport in soil’

by small-scale air turbulence. The turbulent air motion in clouds influences how the raindrops interact, grow in size and distribute in space and how the rainfall occurs. Next time it is windy and raining, look out of the window (or for the full experience, go outside). You might notice that there is a structure to the rainfall, rather than just a steady stream of water coming down. The rain comes down in sheets and bursts, which have a pattern almost like ocean waves. Simulating water particle settling velocities and growth rates in turbulent air conditions is important for understanding these localised features in rainfall.

The way in which air turbulence affects the distribution of droplet sizes and the rate of conversion of these droplets to raindrops is therefore an important topic. Dr Wang and his colleagues have shown that the influence of turbulence can be large, and that it depends on characteristics such as the rate of dissipation of turbulence kinetic energy (how quickly the turbulence transfers energy across scales and converts kinetic energy into heat).

However, simulations of rainfall formation cannot cope with the enormous range in scales involved (sub-millimetre to multi-kilometre). Dr Wang and his team have worked on incorporating the effects of air turbulence on water droplet growth and precipitation rate across many scales, and on the impact of such effects on the dynamics and lifetime of clouds themselves. They found that there are strong variations in the interactions between water droplets and turbulence, with these interactions changing greatly between small and large droplets and between different microphysical processes such as diffusional growth versus growth by collision-coalescence.

Particles in Turbulent Fluid Flow

Normally, the settling rate of small particles in a fluid (such as raindrops in air) is the same as the terminal velocity of those particles, where the forces of gravity and air resistance balance out. However, if the particles are heavy (meaning the particle-to-fluid density ratio is large) and the fluid is turbulent, this may not be the case. Studies since the 1980s have looked at this problem and have shown that particle settling rates tend to be faster than their terminal velocity, with particles accumulating along open pathways within the turbulence. Using rainfall as an example, this could result in ‘sheets’ of rain descending faster than their terminal velocity

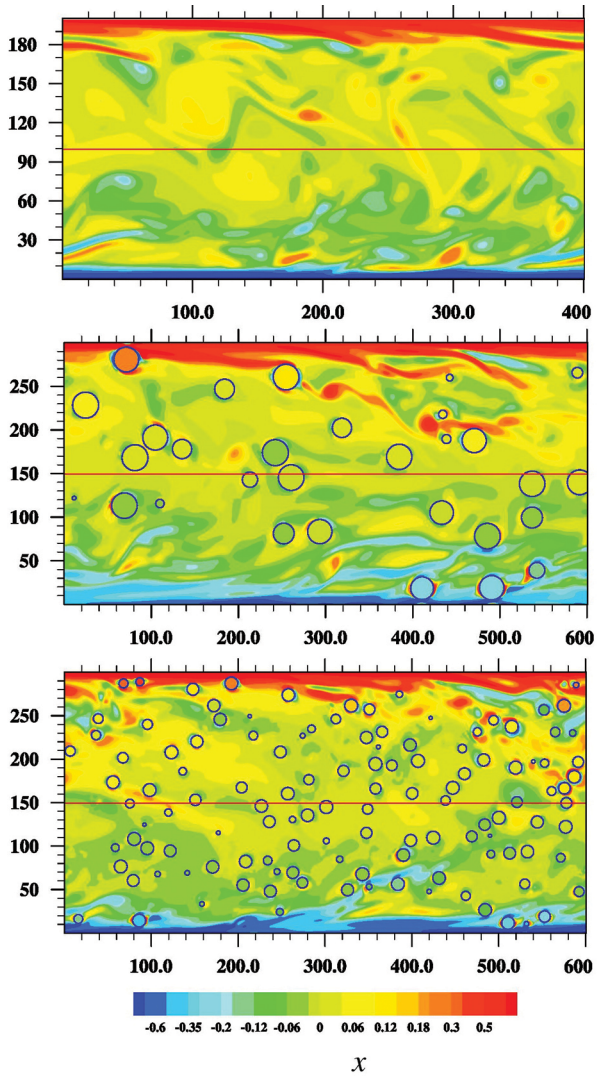
In 1993, Dr Wang and colleagues simulated this situation and showed that this effect can be much higher than previously thought. The greatest difference occurs when the particle response time is similar to the time scale of the smallest vortices in the turbulent flow. However, the organisation of large-scale turbulent vortices can also greatly influence the spatial transport and mixing of particles. An important factor in this is the ‘Kolmogorov scaling of turbulence’, which links the time scale of the smallest vortices to the viscosity (‘stickiness’) and the energy dissipation rate.

Another important factor is that the accumulation of particles in downward-moving channels in the turbulent fluid can have a feedback effect on the structure of the turbulence. If enough particles (such as raindrops) accumulate in one of these narrow channels, then they can dampen certain scales of turbulent motion and reinforce others, altering the spatial and temporal structures of turbulence. Dr Wang’s work has started to demonstrate this feedback effect and others in the interactions between the fluid flow and the particles moving through it.

Many factors such as turbulent motion, particle-particle interaction and particle-wall interaction, control the movement and distribution of particles. Dr Wang has recently been working on simulations of turbulent fluid flow containing particles of different sizes. His team aims to test out a new simulation approach and to explore what happens when different particle sizes are used. In these cases, the particle-fluid interactions cannot be represented in any other way except DNS. For the rainfall example, such particle size-resolved DNS will predict how droplet-droplet hydrodynamic interactions influence the droplet-droplet collision efficiency – a very difficult topic which is currently not well understood. This direction will provide further information about how localised rainfall patterns occur under different atmospheric conditions. This information would allow predictions of small-scale rainfall patterns, which are very difficult to simulate using current models.

Colliding and Growing

Dr Wang’s team also showed that the collision rate of particles, leading to the production of larger particles, is dependent on the nature of the turbulence within a fluid. Using a technique known as Point-Particle based Direct Numerical Simulation (PPDNS), the team was able to simulate this process. In recent years, Dr Wang developed a new method called Hybrid Direct Numerical Simulation (HDNS), which includes the local interactions between colliding particles and their effects on the surrounding turbulent



Instantaneous spanwise vorticity on a 2D slide from 3D particle-resolved simulations in a turbulent channel.

conditions. This enables the team to approximate the collision efficiency – how often the particles moving towards one another actually collide, rather than slipping past one another.

The team's work in this area has opened up new ways to rigorously address the multiscale problem of particle-fluid and particle-particle interactions in a turbulent environment, allowing different physical questions to be addressed and different conditions to be explored. Their new methods allow the mixture of particles and fluid to be simulated much more accurately than before. They have also shown evidence for simulating effects within the two-phase system that have been impossible to simulate previously. This is important, as one of the best ways of knowing that your simulation is good is if it predicts system properties that have been observed, but are not well understood. In some cases, simulations can reveal completely new phenomena that have never been observed, as observing detailed flow structures in a particle-fluid system can often be very challenging due to optical obstruction by particles.

'Warm rain formation' is where rain droplets form in clouds with a temperature above freezing. This is the most common form of droplet formation in tropical and temperate latitudes. The effects of turbulence

on droplet growth through collisions can be crucial in this type of cloud. In fact, Dr Wang's work has shown that specific cloud types (such as cumulus clouds) tend to produce a turbulent in-cloud environment, and therefore, the rainfall droplet formation taking place in them.

Rainfall is not the only process where our understanding has benefitted from Dr Wang's work. Ocean currents can be considered to be multi-phase flows, particularly when water layers with different temperatures and densities interact. In addition, the movement of water through soil is vital for water storage in catchments, and has a strong impact on flooding and plant nutrition through the transport of material. There is no shortage of examples of how this work is important for understanding natural phenomena, such as settling of sediments in rivers, transport of dust from soil erosion or the dispersion of volcanic ash clouds.

In large-scale chemical processes, particle-laden fluid flow is common. Very often, the success of the desired chemical process depends on specific particle densities and distributions within the flow. Getting the conditions right requires simulation and modelling, which can be difficult to achieve with this two-phase system (solid particles in a fluid medium).

Recent work by Dr Wang and his team has involved developing the physical systems to allow massive numerical simulations to take place. This is needed to investigate the complex behaviours seen at small scales by particle-fluid mixtures. One of the ongoing issues is the dynamics of fluid-particle mixtures flowing through rough-walled systems, such as those in industrial devices. This work will have direct commercial applications as it will help engineers better design large-scale industrial technology.

Future Work

Recently, Dr Wang and his team have been working to develop methods that can be applied generally to a wide range of different types of multiphase fluid flow. These include the flow of compressible fluids, or systems containing complex moving boundaries between fluids and solids. If methods can be developed that allow these complex fluid dynamics systems to be simulated, then it will become possible to greatly improve our understanding of a vast range of topics, including atmospheric and ocean flow, soil-water interactions and the behaviour of fluids within complex moving systems such as combustion engines, oil rigs and even volcanoes.

Meet the researcher

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Dr Lian-Ping Wang received a Batchelor's degree in Applied Mathematics and Engineering Mechanics from Zhejiang University, Hangzhou, China in 1984, and spent another two years there working on graduate coursework before coming to the US in 1986. He received a PhD in Mechanical Engineering from Washington State University in 1990, on the topic of the dispersion of heavy particles in turbulent motion. He was then a Visiting Research Associate at Brown University from 1990 to 1992, after which he was a Research Associate at Pennsylvania State University from 1992 to 1994 and an Assistant Professor at the University of Delaware from 1994 to 2001. In 2001 he became an Associate Professor and in 2010 he was made a Joint Professor at the College of Engineering and the College of Earth, Ocean and Environment at the University of Delaware. In 2017, he was appointed a Chaired Visiting Professor at Southern University of Science and Technology, China. He has held numerous additional visiting researcher posts at other research establishments in the USA, South Korea, Japan and China.

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FUNDING

US National Science Foundation
US Department of Agriculture
US Department of Energy
US AFOSR
US National Center for Atmospheric Research
National Science Foundation of China

A BRIGHT FUTURE OF SUSTAINABLE ENERGY

Over two hundred years of intensively burning the Earth's fossil fuel reserves has pushed our planet to the brink of disaster, and the future of our species and that of countless others is becoming increasingly uncertain. Since the Industrial Revolution – that period between the late 18th and early 19th century – humans have been pumping ever increasing quantities of carbon dioxide into the atmosphere, along with other greenhouse gases such as methane and nitrous oxides.

Before this time, carbon dioxide existed in the atmosphere at a concentration of about 280 parts per million (ppm) – this means around 280 carbon dioxide molecules for every million molecules in the air. Shockingly, this value has now risen by around 45% almost entirely due to human activity, up to its current value of about 406 ppm (November 2017).

Our Earth has historically existed in a state of equilibrium – absorbing energy from the Sun, and maintaining a fairly constant average temperature by releasing energy back into space as infrared radiation, with a small amount being absorbed by carbon dioxide and other greenhouse gases in the atmosphere. However, with increasing levels of these gases in the atmosphere, more and more of this infrared radiation is absorbed, trapping heat and disturbing the planet's delicate balance. With a 45% rise in carbon dioxide levels since the Industrial Revolution, and much of this attributed to the last few decades alone, it's no wonder that 16 of the 17 hottest years on record have occurred since just 2001.

Although our carbon dioxide emissions from burning fossil fuels have recently started to level off for the first time, showing very little change between 2014 and 2016, this is no reason for celebration. Let's not forget that our annual carbon dioxide emissions – now about 35 billion tonnes every year for the past three years – are the highest they've ever been. Also, since much of this carbon dioxide remains in the atmosphere, stable emissions mean that the carbon dioxide concentration in the atmosphere still continues to rise.

Therefore, we now need to rapidly switch our fossil-fuel-powered electricity generation, transport and industries to carbon-free energy, such as that provided by wind farms, hydroelectric stations, solar farms and even nuclear energy plants. If we fail to take the drastic action required, our continued warming of the planet will lead to a myriad of disastrous consequences, many of which have already begun, such as melting sea- and land-ice, flooding, droughts, severe weather events, species decline and crop failure.

Thousands of scientists and engineers across the globe are working hard to make this rapid shift to renewable energy a reality, and in this section, we showcase a number of promising research projects. We kick-start this section with a focus on wind power – that underutilised resource that humans have been tapping into for millennia – since the very first sailing boats were used. As a clean, much more sustainable alternative to burning fossil fuels, wind turbines that generate electricity release no greenhouse gas emissions, occupy very little land and consume no water during operation, while taking advantage of a plentiful, renewable and widely distributed source of energy. Although wind energy accounts for still a small fraction of the total global electricity supply today, by 2030, the Global Wind Energy Council predicts that nearly 20% of the world's electricity will come from this renewable resource.

To allow wind energy to realise its maximum potential, turbines need to be placed in locations with favourable weather conditions, and ways to extend their lifetimes must be devised. Also, the way that turbines are arranged within a farm can seriously affect their efficiency, as one turbine can disturb the wind in such a way as to have

a detrimental effect on a neighbouring one. This not only causes significant decreases in efficiency, but this disturbed wind flow (called the 'wake') can also damage turbine components and make them more prone to fail, leading to shorter turbine lifespans and to higher maintenance costs. Therefore, having an increased understanding of these turbine-turbine interactions can help us to design much more efficient and cost-effective wind farms, seriously aiding our quest for a sustainable planet. In the first article of this section, we introduce research led by Dr Glen Whitehouse at Continuum Dynamics Inc., who is developing mathematical tools to model the wakes of wind turbines, to put an end to this uncertainty.

Just like solar energy, which is only available during daylight hours, even the windiest locations often experience periods of calm. Thus, to make the most of these two renewable resources, we must find efficient ways of storing the excess energy that they harness, so that it can be used later and doesn't go to waste. This is an area where lithium-ion batteries are making their mark. Not only do these advanced batteries hold promise for storing energy that can later be used for domestic and industrial purposes, but they also make ideal power sources for vehicles, replacing the need for petroleum-powered engines that contribute to climate change. Indeed, most of today's electric vehicles use lithium ion batteries, and intense research efforts are ongoing across the globe to find ways of making them more energy dense and long-lasting.

This is where the research of Dr Daniela Molina Piper, Dr Tyler Evans, Dr Se-Hee Lee and their team at SiILion Inc. comes in. In the next article of this section, we showcase their work in designing and building highly efficient and cost-effective lithium-ion batteries. These scientists have been rewriting the rulebook on battery design, and so far, their new prototypes are showing huge promise, with energy densities greater than any commercial lithium-ion battery currently available.

A perhaps controversial source of energy that is hotly debated in the world of sustainable energy is nuclear fission. Although energy harnessed from nuclear fission reactions is considered 'clean' by many, as it doesn't produce greenhouse gases that contribute to climate change, whether or not it is 'sustainable' is still open for discussion. For one, there is a finite amount of uranium on Earth, and estimates vary on how much of this we will be able to extract – with supplies lasting from anywhere between a few hundred years to several tens of thousands of years at our current rates of consumption.

Another serious concern surrounding the use of nuclear energy is the harmful nuclear waste that is generated in the process. Nuclear waste is considered to be a major radioactive pollutant, with certain grades of waste remaining dangerous for hundreds of thousands of years, undermining nuclear fission's reputation as a sustainable energy source. Indeed, waste that is graded as 'high level' must be encased in sealed containers and buried deep underground indefinitely. Also, despite all the precautions taken, leaks of radioactive waste into the environment have happened many times throughout history.

If we understood more about the chemical and physical properties of this high level nuclear waste, we could design more effective strategies for treating it, storing it, and even helping to clean it up if a spillage were to occur. That way, we could more confidently use nuclear fission alongside renewable energy technologies to replace fossil fuel combustion, as we attempt to move towards a low-carbon future. Towards this end, many scientists across the globe are working to pin down the behaviour of the radioactive elements found in high level nuclear waste, such as plutonium, and their compounds. In this section of the edition, we meet three research teams who are doing just this.

First up is Dr Thomas Albrecht-Schmitt and his group at Florida State University. Through a series of highly-dangerous experiments, his team has successfully investigated the chemical bonding and structure of molecules containing several different radioactive elements, providing important insight into their chemistry. Their studies could be an important step in designing compounds to safely store or even clean up nuclear waste.

Computational modelling is another important way to investigate the properties of these dangerous substances – and removes the need to handle them in the lab. Next in this section, we meet Dr Kirk Peterson and his team at Washington State University, who are developing computational tools called 'Gaussian basis sets' to create increasingly accurate models of heavy elements, such as those found in nuclear waste.

Our third research team dedicated to mitigating the impacts of any future nuclear waste leakages is Dr Peter Santschi's group at Texas A&M University, who investigate what happens when radioactive elements, such as plutonium and radioiodine, are released into the environment. In this next article, we highlight their research into the mobility of these radioactive substances within the environment – work that is providing the information necessary for assessing the environmental and human risks posed by these contaminants.

While nuclear fission involves splitting heavy atoms into smaller fragments, and releasing energy in the process, nuclear fusion is essentially the opposite – taking very light elements such as hydrogen and fusing them together into heavier elements such as helium, by subjecting them to extremely high temperatures and pressures. Overall, this process releases even greater amounts of energy that nuclear fission – four times more per kilogram of fuel – and produces no toxic by-products. Although this process happens with ease under the extreme conditions inside stars such as our Sun, or upon detonation of a hydrogen-bomb, scientists have yet to achieve a controlled nuclear fusion reaction that gives more energy out than the amount put in to initiate the reaction.

Therefore, many research teams across the globe are working hard to achieve a controlled nuclear fusion reaction that can sustain itself, so that the heat produced could be harnessed to turn a turbine and generate electricity. One such research team is Setthivoine You's group at the University of Washington, who are taking inspiration from astrophysical jets – columnated flows of plasma (ionised matter) that extend from black holes and other rotating astronomical phenomena. Our next article showcases the team's 'Mochi.Labjet Project', which aims to recreate these astrophysical jets in the lab for the purposes for attaining nuclear fusion here on Earth.

Also in the race for fusion is Dr Michael Brown and his team at Swarthmore College, who are working on a project known as the Swarthmore Spheromak Experiment (SSX). To conclude this section on sustainable energy, we highlight their research into a process known as magneto-inertial fusion – a totally new approach to fusion energy, which relies on generating small parcels of hot plasma that can then be compressed, hopefully initiating the fusion reaction.

CATCHING THE WIND: UNDERSTANDING THE DYNAMICS OF RENEWABLE ENERGY

As renewable energy sources such as wind, wave, and solar become more ubiquitous, the importance of understanding the detailed mechanisms of their operation is essential. In particular, with a dynamic and turbulent energy source like wind, an accurate way of modelling the flow and interaction with the wind turbine is highly desirable. **Dr Glen Whitehouse** and the team at Continuum Dynamics Inc. have been developing innovative ways to do just this.

The pressing issue of climate change, and the urgency to decrease our reliance on fossil fuels has sparked major developments in the clean energy industry, including the advancement of technology to harness wind power. As of 2016, the power globally generated from wind sources exceeds 450,000 megawatts, and the Global Wind Energy Council predicts that by 2030, nearly 20% of the world's electricity will come from wind power alone.

The typical way in which wind energy is harnessed and electricity generated industrially is with a turbine. For wind turbines to be successful as an energy provider, the energy they yield must be maximised with favourable weather conditions, while operating costs must be minimised. As such, largescale arrays of turbines in a wind farm are preferred as they address both of these issues. However, other issues can arise from having several turbines arranged in a wind farm due to the flow of wind around the turbines becoming disturbed, resulting in turbine-turbine interactions.

The flow of wind through turbines induces forces on the structure, referred to as the 'aerodynamic loading', and much research has been undertaken to clarify the effect these loads have on the blades. The region of disturbed flow behind the turbine as the wind interacts with blades is known as the 'wake'. This interaction between the wake from one turbine on the aerodynamic loading of another results in a significant decrease in their efficiency. Not only this, but the interactions between turbines and wakes results in components fatiguing and becoming prone to fail, which leads to higher maintenance costs.

Who are Continuum Dynamics Inc.?

The research led by Dr Glen Whitehouse, Associate at Continuum Dynamics Inc., aims to put an end to the uncertainty surrounding current turbine analysis, by accounting for the intricate and complicated interactions of turbine blades in a cost effective first-principles manner. Continuum Dynamics Inc. was founded in 1979 as an engineering research and development company and service provider for government and industry, and they have expertise in a variety of areas related to fluid dynamics and fluid-structure interactions. Continuum Dynamics Inc. is also a world recognised authority on the unsteady aerodynamics of rotating machinery and wake vortices.

The main aims of Continuum Dynamic Inc. is to provide high-quality, cost-effective engineering services, and state-of-the-art technical solutions for government and industry. They have undertaken a wide spectrum of business activities including, contract research, software development and licensing, engineering and design services, smart materials and robotic systems development, and testing services. Their government and commercial customers come from a range of industries including: aerospace and defence, electric power generation, forest management, agrochemical application, and pharmaceuticals.

‘Continuum Dynamics Inc., in collaboration with Professor Marilyn Smith at the Georgia Institute of Technology, is developing an advanced, hardened, efficient easy to use suite of high-performance computing software for predicting wind turbine/ farm aeromechanics in the industrial environment’

CREDIT: Christian Steiness/Vattenfall

Prediction Problems

When trying to predict the behaviour and nature of flow around objects, where possible, wind tunnel experiments are used to give accurate insights. However, these methods are costly, and in the case of larger structures, cannot be readily scaled-up. On top of these limitations, wind tunnels also don’t account for other atmospheric conditions – therefore, for assisting the design of commercial sized wind farms, this method is impractical.

Currently, the computational design tools that are used to predict and optimise the performance of wind turbines only work for individual turbines. Dr Whitehouse explains that ‘contemporary design tools fail to account for the unsteady fluid structure interactions that drive costly fatigue’. They don’t take into account any of the turbine-turbine wake interactions that occur in reality, nor the unsteady stress and strain the components are subsequently put under. Therefore, predictions of the potential power that a wind farm can generate are usually overestimated. Often, these calculations are compensated by broadly imposing a 20% reduction factor. Yet occasionally, even this gross simplification still overestimates the power generated. This uncertainty surrounding the power output for wind turbines and the potential underperformance poses problems if wind turbines are going to be heavily invested in.

There are methods that use high performance computing, which will accurately account for these turbine-turbine interactions, but rely on a compromise between the accuracy of the calculation and the high expense and time required to perform. Accurate and high resolution models of aerodynamics require very large scale computations, and even when this is achievable, the complexity and cost of these methods means that their usefulness is limited. ‘Unfortunately, such tools require dedicated experts to generate reliable predictions and are too complicated and expensive for industrial use,’ says Dr Whitehouse. When applied to simulate real-world wind farms, modelling the wakes from turbine to turbine is so complex that it requires the latest high performance super-computers.

A Potential Solution

To combat this problem, Dr Whitehouse and Continuum Dynamics Inc., in collaboration with Professor Marilyn Smith and her graduate students at the Georgia Institute of Technology, are developing an advanced method for predicting the aeromechanics of wind turbines and farms. They do this by taking the best aspects of high-performance computing methods, and make them adaptable to industry.

A significant barrier that hinders the application of these high-performance computer calculations to any commercial adaptation is that that the software used is unique and cannot be adapted or reused in an industrial setting. Continuum Dynamics Inc. is developing software with a standardised user interface that no longer requires a dedicated team of experts to operate.

The benefit of this industrially applicable software is that it could be used in many multidisciplinary areas of wind turbine design and analysis. The tools that Dr Whitehouse and Continuum Dynamics

Inc. are creating will directly address the current limitations of predicting unsteady loads on wind turbine blades, and other real-world conditions. The team's software is also being applied to other applications, such as helicopters.

Pioneering Results

In order to address the difficulties in modelling the flow of wind (also known as computational fluid dynamics), Dr Whitehouse, Continuum Dynamics Inc. and the Georgia Institute of Technology have recently developed a unique hybrid approach. This approach makes use of a piece of open source government software from NASA called 'FUN3D'. This software has the ability to predict the flow of wind near the turbine (including the turbine blades and its tower), and was coupled to software developed by Continuum Dynamics Inc., VorTran-M, to predict the wind turbine's wake. This integrated solution was then coupled further with a computational structural dynamics code which is able to predict any deformation that would occur in the turbine's blades. This approach is completely unique, and because it accounts for the downstream wake from the turbines, it means that computational effort can be focussed on the regions of interest. In this way, detailed predictions of the turbine blade performance can be made at a fraction of the cost of traditional high performance computing methods.

These innovative methods were then applied to various problems that result from wake-based interactions. Key successes from these studies include the accurate prediction of fluid dynamics phenomena known as 'vortex rings' using more than an order of magnitude less computing power than traditional methods. Additionally, unsteady wind turbine aeroelasticity was successfully simulated with less than 50% of the computational cost usually required by traditional high-fidelity numerical solvers, such as FUN3D applied without VorTran-M.

Public Benefit

The potential of the team's pioneering computational method for modelling wind turbine wakes is that an easy-to-use system would be in place to design and analyse robust new turbines. These turbines would have increased performance and lifetime, reducing the costs of wind farm projects. Also, the team's modelling would lead to quieter turbine designs and a reduction in the maintenance costs, which would encourage their integration into communities.

Integrating wind farms into communities is hugely advantageous as they greatly benefit local economies, particularly in rural areas where the majority of the most efficient land-based wind sites are found. The design of modern wind turbines is such that farmers would still be able to work the land as the acreage turbines use is minimal. As well as this, the landowners receive additional income from the wind farm's owners.

Another concern is the interaction of the wind turbine wakes with power lines. These wakes can sometimes induce an adverse phenomenon known as galloping, where the power lines can be damaged or broken. In this assessment, distances of more than a mile between the wind turbine and power lines may need to be modelled.

Finally, the ability to accurately predict wakes at low computational cost and over long distances would enable offshore wind farms to be analysed in greater detail than current methods. Precise prediction and analysis of offshore wind farms is especially important, as any maintenance that would be required is far more difficult to carry out compared to land-based turbines.

Future Prospects

Because of the complexity of a system that takes into account atmospheric conditions, the flexibility of the rotating blades, and the flow field induced by neighbouring turbines in a wind farm, the integrated software by Continuum Dynamics Inc. is being updated. 'Continuum Dynamics Inc. is currently halfway through the two year United States Department of Energy sponsored research and development effort, and is now focusing on software integration, debugging and testing,' Dr Whitehouse tells Scientia. The CDI-GT team is aiming to improve their software by hardening the interface, making it generally more robust, and by improving the usability and functionality. Dr Whitehouse also mentions that 'the next steps are to commence with deployment and testing of the software by partners in the wind industry and in other industries interested in vorticity dominated flows and rotary-wing aeromechanics'.

Ultimately, a major goal of these developments is to work towards making the wind power more cost competitive than conventional energy sources. Despite the cost of wind power decreasing dramatically over the previous decade, the technology and infrastructure still require a larger initial investment than fossil-fuel generators. The importance of the team's work is that by predicting the uneven aerodynamic loading on the turbine blades, superior and more robust wind farms can be designed with lower maintenance costs. This will drive down the cost of investment in the long run. Not only this, but if the efficiency of wind farms could be accurately predicted at low cost and computing power, investors would be far more drawn to them as an alternative energy source to begin with.

Meet the researcher

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Dr Glen Whitehouse is an Associate with Continuum Dynamics, Inc. He received his BS degree in Aeronautical Engineering from Clarkson University in 2000 and his PhD and DIC in Aeronautics from Imperial College London in 2004. While at Imperial College, he gained extensive experience modelling rotor aeromechanics and wake dynamics with both traditional inflow based analysis codes and high fidelity CFD techniques. The UK government's Engineering and Physical Sciences Research Council described his doctoral work as 'internationally leading'. Dr Whitehouse's later research focused on predicting rotor performance in and out of ground effect and during wake interactions. He has authored or co-authored of over 90 technical reports and papers related to rotary-wing research and development. Dr Whitehouse has been a member of the Aerodynamics Committee of the American Helicopter Society since 2005, and was the Chair from 2012 until 2014. He is an Associate Editor of the Journal of the American Helicopter Society, and was the Technical Chair for the 2016 Annual Forum of the American Helicopter Society.

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FUNDING

U.S. Department of Energy under award number DE-SC0004403
U.S. Department of Energy under award number DE-SC0013231

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Continuum Dynamics, Inc.

THE HIGHEST ENERGY LI-ION BATTERY: UNLOCKING THE POTENTIAL OF THE SILICON ANODE AND NICKEL-RICH NMC CATHODE

Over the past decade, lithium-ion batteries have become essential to the portable electronics industry, and more recently have been championed as the transportation power source of the future. However, if electric vehicles are to gain widespread commercial success, modern lithium-ion batteries need to be cost effective, energy dense and long-lasting. **Dr Daniela Molina Piper, Dr Tyler Evans, Dr Se-Hee Lee**, and their team at SiILion Inc. have been completely rethinking the fundamental building blocks of these typical batteries, in order to develop an elegant solution to a significant modern problem.

A lithium-ion battery essentially consists of three components: two electrodes, and an electrolyte solution between them. The basic principle is that lithium ions contained within the electrolyte move from the positive electrode (cathode) to the negative electrode (anode) when the battery is charging, and back again when discharging. Almost all commercial lithium-ion batteries use an anode made primarily of graphite, long regarded as the most efficient material in its ability accept and release lithium ions during battery charging and discharging. The effective capacity of the battery is determined by the number of lithium ions that can reversibly travel between the anode and cathode material throughout battery operation.

The success of the lithium-ion battery is due to its many advantages over other contemporary batteries. Lithium-ion batteries have an almost negligible 'memory effect' (also known as the 'lazy battery effect') – a phenomenon that causes the battery to lose its ability to store charge (or its 'capacitance') with repeating recharges over time. They also have a large 'energy density', meaning that they have a high energy yield per unit volume of battery material. Additionally, they have low 'self-discharge' – a phenomenon whereby the stored charge in a battery becomes reduced, even when no device is connected to the electrodes.
To significantly reduce our carbon emissions, and thus mitigate the most disastrous consequences of climate change, replacing our gasoline-powered cars with battery-powered ones is an essential step. The lightweight nature of lithium-ion batteries, as opposed to a hefty lead-acid battery, make them an attractive option for this application. Indeed, most electric vehicles currently in development rely on a lithium-ion battery as their power source. However, the main problems that are incurred come down to battery capacity and longevity – the battery simply not having enough energy to power long journey distances. In order to be fully adopted as a viable transportation solution, the agreed estimate is that batteries need a gravimetric energy density of over 350 Watt-hours per kilogram (Wh/kg). Best efforts of current lithium-ion batteries fall far short of this, below 300 Wh/kg.

A Change for the Better

Over the past 25 years, incremental design improvements have allowed lithium-ion batteries to increase their energy density by around 5–6% each year, but since their inception, the basic materials used in these batteries have remained unaltered. This slow improvement in performance is underwhelming, and the team at SiILion believes that this adherence to the same stale electrode materials is holding back the growth of the industry. A drastic break with the status quo in lithium-ion materials is needed if the exciting future adaptations predicted for lithium-ion batteries are to be achieved anytime soon.

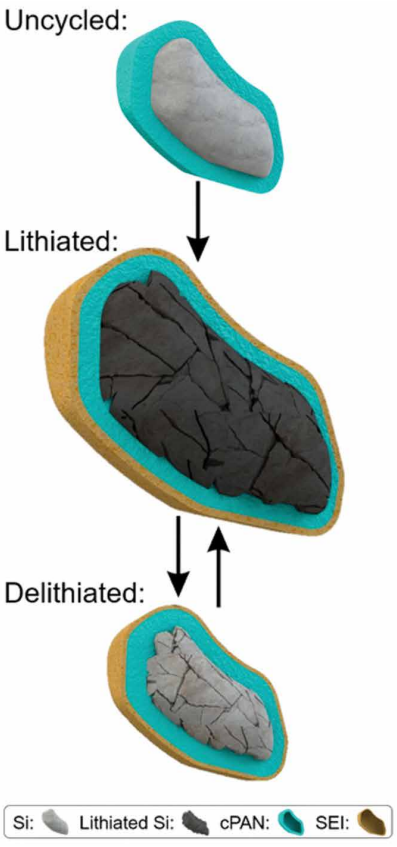

Image of SiILion's proprietary micron-Si enabling mechanism

'SiILion can integrate a wide range of silicon materials into its anode, to adapt to performance needs, and this also allows the SiILion cell design to realise the improvements that will arise due to new material introduction into the lithium-ion industry' – Dr Molina Piper

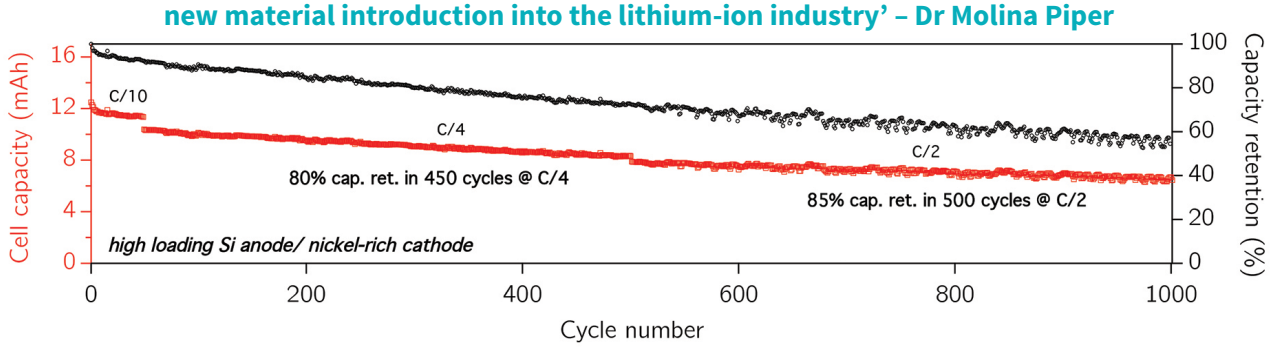

Figure highlighting SiILion's cycling capability

Silicon anodes could be a suitable candidate to kick off this paradigm shift in lithium-ion batteries. In theory, silicon is an ideal replacement for graphite because of its low working potential versus lithium and high specific capacity, which is nearly 10 times higher than the most modern graphite anodes. As such, considerable research has been undertaken with the goal of creating a lithium-ion battery with a functioning silicon anode. However, in practice, a silicon anode has several drawbacks, particularly with its propensity to expand when the battery is charged.

The volume expansion of graphite anodes in most commercialised batteries is between 10–13%, while silicon's expansion can be almost up to 300%. This expansion problem causes massive structural damage in the battery and compromises the fragile interface between the solid silicon electrode and the liquid electrolyte (the 'solid-electrolyte interphase', or SEI). Most modern research focuses on modifying the silicon material in a complicated way to accommodate more lithium ions without such severe expansion. The drawback of these modifications, however, is that they require intricate and costly processing methods, making this approach less appealing in the manufacture of commercial batteries. As Dr Evans of SiILion Inc. explains, 'most of the published work around silicon anodes focuses on complex material modifications that ultimately will introduce manufacturing processes which are very difficult to scale'. A simple, scalable solution to the silicon anode is one key to higher performing batteries.

But What About the Cathode?

By improving the anode's performance, you can increase a battery's maximum energy output by 20–30%. However, in order to unlock the true potential of the battery, the cathode needs to be similarly enhanced. In terms of the cost of producing lithium-ion batteries, the cathode accounts for 30% of the total expense – more than twice that of the anode. Most conventional lithium-ion batteries use expensive and toxic cathodes, containing large amounts of cobalt, limiting their widespread application to electric vehicles.

Thus, cathodes containing large proportions of nickel are being explored as alternatives. Unfortunately, they are also problematic in the sense that they can be unstable at high temperatures and their structure may not be adequately robust. So, similar to the silicon anode, modern research is focusing on expensive and elaborate modifications to these nickel-based cathodes, which again will limit their commercial viability.

A Revolutionary Approach from SiILion Inc.

Dr Molina Piper, Dr Evans, Dr Lee, and their team at SiILion Inc. see the potential of these next-generation electrode materials, but also believe that the complex modification of the cathode and anode is not practical if these materials are to be applied to commercial battery systems. They claim that this method of combining next-generation materials with old-generation electrode and electrolyte designs, leads to obvious incompatibility issues. Because of this, the materials are increasingly over-engineered, while very little practical progress is made.

The team at SiILion is beginning to rewrite the rulebook for lithium-ion battery design. Not only do the cathode and anode materials need to be next-generation, the entire battery also needs revamping. They are shifting their focus to auxiliary battery materials, building a support system for the modern silicon and nickel-rich electrodes using unique electrolyte compositions and electrode binders, while maintaining the advantage of decades of manufacturing expertise by premising their designs on compatibility with existing lithium-ion battery manufacturing methods. As Dr Molina Piper explains, 'enabling the next-generation electrode materials will mean enabling a next-generation lithium-ion system design'. Moreover, the strategy for attaining next-generation performance must be commercially viable. SiILion's cell technology, through utilisation of lower cost materials and manufacturing compatibility, will be 30% less costly ($/kWh) than state-of-the-art lithium-ion cells. By approaching the problem from the view of the battery cell system, SiILion achieves its breakthrough energy density and performance.

Promising Results

With this philosophy in mind, the team at SiILion has undertaken the task of redesigning the old lithium-ion battery system, and their approach has already revealed some impressive achievements. SiILion has shown that when integrated into their unique system, state-of-the-art 'nickel-rich' cathodes and silicon anodes demonstrate a much-improved structural stability and safety, even at high temperatures. Dr Molina Piper also says that 'SiILion has created the first viable 80% (by weight) silicon lithium-ion battery anode, capable of integration into standard electrode manufacturing processes'.

In fact, every silicon material that has been implemented into the SiILion system has shown an improvement in performance. 'SiILion has worked with over two dozen types of silicon active materials (from over

‘Most of the published work around silicon anodes focuses on complex material modifications that ultimately will introduce manufacturing processes which are very difficult to scale’ – Dr Evans

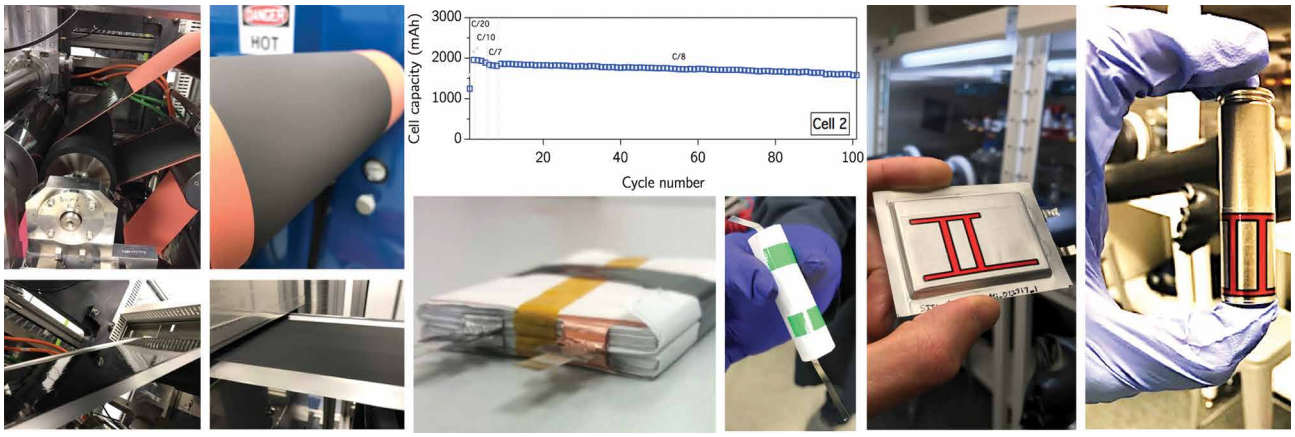

Figure highlighting SiILion’s scaling capability

one dozen vendors), all showing marked improvement in capacity retention and coulombic efficiency when used in SiILion’s anode systems, regardless of the size or shape of silicon particles’ says Dr Evans. Of course, the team has its preferred material candidates, based on material stability and availability at scale. This ability to turn so many commercially available silicon materials into effective anodes could send shockwaves through the industry, making the current, over-engineered silicon anodes look overpriced by comparison.

The exact details of SiILion’s battery design remain confidential, but the problematic expansion effects that plague modern silicon anodes appear to have been overcome. As Dr Evans stated, the anodes display a minimal decrease in capacity after hundreds of charging and discharging cycles, and exhibit high ‘coulombic efficiencies’ – meaning that the charge is reversibly and effectively transferred through the system. This efficiency has been tested and proven with a variety of electrolyte materials, including coveted non-flammable electrolytes, which also shows the flexibility of the SiILion system.

Potential Applications

The real strength of SiILion’s battery system is its simplicity and its ability to be customised. The SiILion anode design can be employed with conventional electrolyte materials and a range of cathode materials, or can be employed with non-flammable electrolytes and next-generation, high-energy cathode materials. Crude, low-cost silicon materials, such as large particle ‘micron’ silicon materials can be incorporated, or more exotic anode active materials, such as silicon nano-wires or nano-featured silicon/carbon composites, could be employed when the system requires higher power with faster charging capabilities. SiILion’s major focus lies on pairing its anode designs with ionic liquid electrolyte materials that can be used for applications that need the highest energy density with an emphasis on the utmost degree of safety.

The team at SiILion particularly stresses the high emphasis they put on safety when designing their next-generation lithium-ion batteries. As anyone who is aware of the Samsung Galaxy Note 7 fiasco can attest, malfunctions involving lithium-ion cells have the potential to be catastrophic. If a faulty battery was scaled-up to the sizes required for electric vehicles, the consequences of malfunctioning would be even greater. With this in mind, SiILion’s use of a non-flammable electrolyte aims to eliminate the stigma that is associated with upscaling lithium-ion batteries to electric vehicle proportions.

In addition to the system’s versatility to accommodate the needs of various applications, the technology was specifically designed by SiILion so that it could be readily integrated into the existing infrastructure that is currently used to mass-produce lithium-ion batteries. This drastically reduces any costs that would be incurred for updating the current hardware, and makes the prospect of using this system commercially all the more attractive.

What the Future Holds for SiILion

‘The SiILion team members have become experts in cell design around high loading silicon anodes, and this has proven very valuable,’ Dr Molina Piper states. ‘SiILion can integrate a wide range of silicon materials into its anode, to adapt to performance needs, and this also allows the SiILion cell design to realise the improvements that will arise due to new material introduction into the lithium-ion industry.’

So, building on their experience and expertise, SiILion’s next endeavour will be to optimise the material properties in their system, and then scale up the technology to truly demonstrate its value for the needs of electric vehicles and other applications. The company is now manufacturing 2.5 Ah prototypes, capable of achieving >300 Wh/kg, a pre-requisite step to ensuring that SiILion’s technology is inserted successfully into the markets. SiILion has also worked with its suppliers and manufacturing partners to validate its claims of lower cost, projecting a 25–35% cost saving, on a $/kWh basis, relative to current technologies.

Along the way to enabling vehicle electrification, SiILion is targeting the application of its technology in unmanned vehicles, specialty applications, and consumer electronics, with its current generation of prototypes designed to meet the requirements of these markets. With its business development efforts led by acting-CEO Mr Ed Williams, SiILion’s first generation prototype technology is under evaluation or requested for evaluation by numerous lithium-ion manufacturers and end-users active in its target markets. Ultimately, through development projects already underway and in the pipeline, SiILion is targeting a battery prototype that is predicted to deliver roughly 390 Wh/kg – far greater than any commercial lithium-ion battery currently available, and tantalisingly close to the energy density stated as optimal for electric vehicle applications.

Meet the researchers

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Dr Daniela Molina Piper leads SiILion's early-stage operations as President and Chief Operating Officer. This includes fundraising, staffing, facilities establishment, day-to-day operations, contracts and project management, prototype development and design, and R&D. She obtained her PhD in Mechanical Engineering from the University of Colorado, Boulder, with her graduate research focused on silicon anodes for next-generation lithium-ion batteries, research that became part of SiILion's core technology. Dr Molina Piper brings a unique blend of industry, academic, and National Laboratory experience to her role at SiILion.

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Dr Tyler Evans leads early-stage operations for SiILion as Chief Technology Officer. Responsibilities include fundraising, staffing, facilities establishment, day-to-day operations, contracts and project management, prototype development and design, and R&D. Dr Evans obtained his PhD in Mechanical Engineering from the University of Colorado, Boulder, and is a co-inventor of the SiILion technologies. Dr Evans' research expertise focuses on enabling next-generation lithium-ion electrode materials by using advanced electrolytes.

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FUNDING

Angel Seed Fund
U.S. Department of Energy: SBIR Phase I, SBIR Phase II
U.S. National Science Foundation: SBIR Phase I
U.S. Department of the Navy: SBIR Phase I
Colorado Office of Economic Development and International Trade (COEDIT): AI ESCR grant
Asia-based automotive OEM: prototyping fund

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SiILion

THE EXOTIC CHEMISTRY OF THE HEAVIEST ELEMENTS

Relatively little is known about the chemical reactivity of radioactive elements, as using them in the lab requires heroic efforts. However, **Professor Thomas Albrecht-Schmitt** and his group at Florida State University have successfully been able to investigate the chemical bonding and structure of molecules containing radioactive elements such as plutonium and californium, providing important insight into their chemistry. These investigations could be an important step in designing compounds to help clean up nuclear waste.

Heavy Chemistry

Since it was first published in 1869, the Periodic Table has seen the addition of many new elements. In the last seventy years, most of these new elements have been in the final two rows of the Periodic Table – home to the heaviest elements known as the lanthanides and actinides.

Today, the Periodic Table contains 118 confirmed elements, organised by the number of protons each element has. The table is then divided into groups, where elements in the same group typically exhibit similar chemical reactivity. For example, Group 18 – a column in the table that contains elements including helium, neon and argon – is nicknamed the 'noble gases' group, as all of the elements in this category are unreactive, colourless gases.

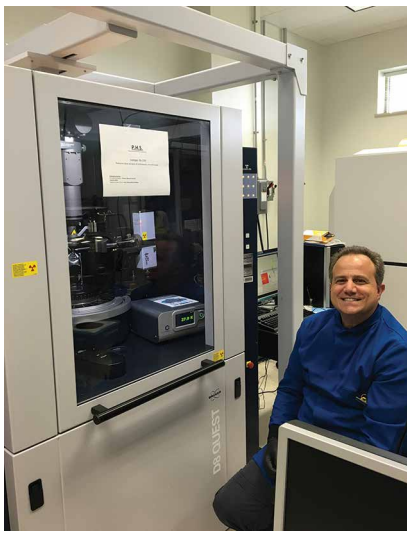
The rows of the Periodic Table are known as chemical series, and there are two chemical series that are separated from the main bulk of the Periodic Table. These are the lanthanide series and the actinide series, home to the heaviest elements of the Periodic Table and including uranium, neodymium and plutonium. Although they are perhaps not the most well-known of the chemical elements, naturally-occurring lanthanide elements are surprisingly common in every-day life. Every smartphone contains a number of different lanthanide elements, which are also known as rare earth metals. Examples include terbium and dysprosium – both of which are important in the colour displays of a smartphone.

Despite their proximity to the lanthanide elements in the Periodic Table, the actinide series of elements differ greatly from their naturally-occurring neighbours. Of the actinide elements (or simply 'actinides'), only uranium and thorium occur naturally in substantial quantities. The rest of the actinides are synthetic, created in nuclear reactors by bombarding naturally-occurring heavy elements with neutrons. Both the synthetic and naturally-occurring actinides are radioactive, and have 'half lives' (the time it takes for half of the atoms in a sample to radioactively decay) ranging from minutes to billions of years.

Relatively little is known about how both the lanthanides and actinides react with other elements and molecules, particularly as their radioactive nature makes them incredibly difficult to work with. Without this knowledge, it is very difficult to devise ways to trap and remove radioactive lanthanides and actinides from nuclear waste. However, Professor Thomas Albrecht-Schmitt and his research group at Florida State University are uniquely equipped to apply conventional investigative chemical tools to these heavy elements, and provide some of the first insights into the chemistry of one of the most exotic regions of the Periodic Table.

Chemical Investigations

Professor Albrecht-Schmitt and his team are experts in investigating the chemistry and bonding of the actinides. They are working at one of the few research institutes in the world where scientists can use sufficiently large amounts of these radioactive elements to synthesise new molecules from them, and probe their properties.



To investigate the electronic structure and reactivity of such elements, Professor Albrecht-Schmitt and his group use a huge variety of both experimental and theoretical methods. Previously, they have focused their attention on understanding the chemical bonding in californium borate, one of the very few molecules containing californium that has been created to date. This molecule (or 'compound') is an excellent model for understanding the similarities and differences between the actinides.

As californium is not a naturally occurring actinide, there are only very small amounts of it in existence. However, the results obtained by Professor Albrecht-Schmitt's team during

‘What makes this discovery so interesting is that the material – rather than being really complicated and really exotic – is really, really simple. Your imagination goes wild, and you think “Wow, I could make that class of compound with many other types of heavy elements”.’

their californium borate experiments were truly surprising and remarkable. By using common chemical structure identification techniques, such as crystallography, they were able to deduce the arrangement of the atoms in the compound. Also, using a series of spectroscopic tools, such as UV-vis absorption spectroscopy, along with computational simulations, the team found that californium atoms were bonded to oxygen atoms in a way that was far more similar to the type of bonding seen in molecules containing transition metals (a group containing iron, cobalt, gold and lead). It was highly unusual to find an actinide element exhibiting this type of chemical bonding.

Previously, it had been assumed that there would be a great deal of similarity in how all of the actinides bonded, as is the case for most other regions of the Periodic Table. However, in the team’s compound, not only was californium bonding in a way that was completely different to what had been seen in other actinides, such as plutonium, americium and curium, but the compound also shown to be highly resistant to radiation damage, making it a possible candidate for use as a nuclear waste storage material.

The team also performed studies using similar techniques on similar compounds called berkelium dipicolinate and berkelium borate. Although there are some similarities between the structures of californium borate and berkelium borate, the team showed how berkelium’s electronic properties, which determine how the element will react, are much more similar to that of the lighter actinides than its nearest neighbour, californium. This was yet another surprising observation in this strange region of the Periodic Table.

Going Nuclear

Illuminating the electronic structure and bonding of these heavy element compounds has another implication for making our nuclear energy safer – it can help us to devise ways to trap and remove these types of compounds from our nuclear waste. Towards this goal, Professor Albrecht-Schmitt and his team have been investigating compounds containing plutonium – a common component of nuclear waste. This project has been supported by a grant from the Department of Energy to form a new Energy Frontier Research Center that will focus on accelerating scientific efforts to clean up nuclear waste.

With a rising global population, it is proving challenging to find viable approaches to meeting our increasing energy needs while also considering the disastrous environmental impact of many energy

sources, such as fossil fuels. While renewable energy sources such as wind and solar power are very attractive options for future investment, such methods cannot always meet our energy demands around the clock. Nuclear power offers an attractive addition to this, as it provides a continuous energy source. However, one of its most serious long-term downsides is the resulting nuclear waste, which can continue to emit significant levels of radiation for thousands of years.

The problem with radioactive waste is twofold. While the radioactive decay of a single atom may be relatively well understood, the chemistry of the complex 'chemical soup' that is nuclear waste poses a far greater challenge. The composition of the waste also evolves over time, with different elements and compounds having different lifetimes. Professor Albrecht-Schmitt and his team hope that their research will lead to the development of new methods for separating different radioactive elements, helping with the capture, clean up and recycling of nuclear waste.

The Secret Life of Plutonium

To gain a deeper understanding of the how radioactive elements might behave in nuclear waste, the team created a plutonium compound – what they call a 'plutonium-organic hybrid'. 'In order to develop materials that say trap plutonium, you first have to understand at the most basic level, the electronic properties of plutonium,' Professor Albrecht-Schmitt explains. 'So that means making very simple compounds, characterising them in exquisite detail and understanding both experimentally and theoretically all of the properties you're observing.'

Using a similar arsenal of techniques to their previous studies on californium borate, Professor Albrecht-Schmitt and his team discovered that an electron was able to hop between two plutonium atoms in their plutonium-organic hybrid compound. This type of electron motion, which is very common in transition metal compounds, had never been observed in a plutonium compound.

Before they had even analysed the compound, the team knew that it would have unique electronic behaviour because of its unusual brown colour. 'Plutonium makes wild, vibrant colours. It can be purple, it can be these beautiful pinks. It can be this super dark black-blue,' Professor Albrecht-Schmitt explains. 'This compound was brown, like a beautiful brown chocolate bar. When we saw that colour, we knew something was electronically unusual about it.'

When the negatively-charged electrons shuttle between the plutonium atoms in the compound, the total amount of charge on each atom changes. This charge on each plutonium atom is what's known as its 'oxidation number' and this strongly determines its chemical behaviour. 'What makes this discovery so interesting is that the material – rather than being really complicated and really exotic – is really, really simple,' says Professor Albrecht-Schmitt. 'Your imagination goes wild, and you think "Wow, I could make that class of compound with many other types of heavy elements".'

The team's discovery deeply increases our understanding of plutonium's chemical behaviour, challenging all previous assumptions about the element. In the future, this information will be invaluable for figuring out efficient ways to trap and remove this dangerous element from nuclear waste.

Looking Forward

Professor Albrecht-Schmitt is the director of the Center for Actinide Science and Technology (CAST) at Florida State University that is dedicated to bringing together interdisciplinary teams from across the sciences to pioneer new ways of understanding some of the most challenging chemistry in the Periodic Table. Already, the work being done here has revealed invaluable information about behaviour and bonding in actinide elements, challenging many previous assumptions. From designing safer waste materials, to creating compounds that can trap and remove hazardous radioactive elements, their work is contributing to a future of safer nuclear energy.

Meet the researcher

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Professor Thomas Albrecht-Schmitt holds the Gregory R. Choppin Chair in Chemistry at Florida State University and is the director of the Center for Actinide Science and Technology (CAST), a Department of Energy, Energy Frontier Research Center – a collaboration between seven universities and national laboratories in the US dedicated to actinide chemistry, materials, and physics. He completed his BSc at Southwest Minnesota State University, before pursuing both his MSc and PhD at Northwestern University, which he completed in 1997. His current research interests are focused on the synthesis, structure elucidation, spectroscopy, and structure-property correlations in heavy element materials.

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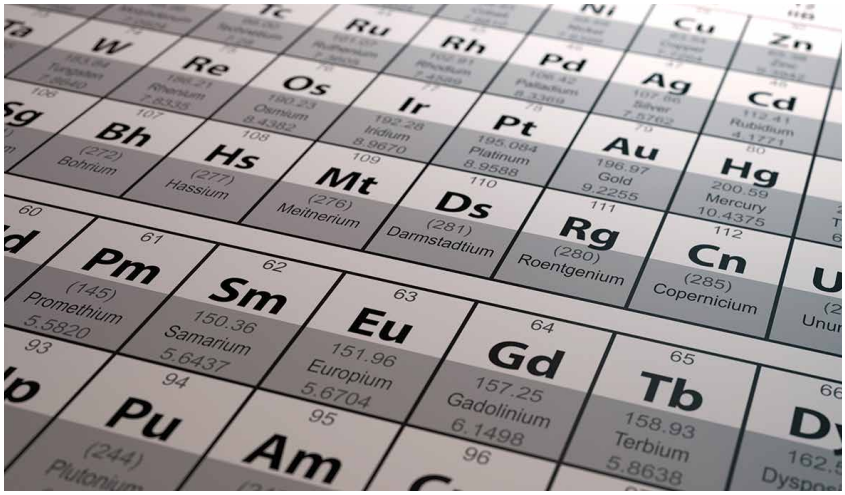
IN SILICO CHEMISTRY: MODELLING THE REACTIONS OF HEAVY ELEMENTS

Is it possible for computational modelling to become sufficiently accurate as to replace experiments? This is one of the many questions that **Dr Kirk Peterson** and his team at Washington State University are working towards answering. As a world-leader in developing Gaussian basis sets for creating increasingly accurate models for the heaviest elements in the Periodic Table, Dr Peterson and his colleagues are finding new approaches for understanding the chemistry and properties of some of the most exotic elements.



What Is *in silico* Chemistry?

In recent years, computational modelling has become a commonplace technique for trying to understand the intricacies of chemical reactions. Recent advances in experimental laser technologies are approaching the stage where it is possible to make a full 'molecular movie' of a chemical reaction, where information on the positions of all the atoms at all points during the reaction can be obtained. However, this is far from a mature technology. This means that a complete understanding of chemical reaction mechanisms is often only possible through computationally modelling the system of interest.

Computational modelling is a powerful tool for obtaining information that cannot be obtained experimentally, and is often crucial for understanding the rationale behind experimental observations. There are many advantages to using computational models to study chemical reactions, rather than direct experimental measurements. For investigating reactions that may pose significant health hazards, computational modelling is an infinitely safer alternative. Furthermore, certain chemicals may be very difficult to prepare, or the species may only exist transiently, making it very challenging to make experimental measurements. Computational modelling offers a much more affordable and reliable alternative for studying many chemical species, and can be used as a screening technique for identifying which chemical systems are likely to have useful properties or be interesting for further experimental investigation.

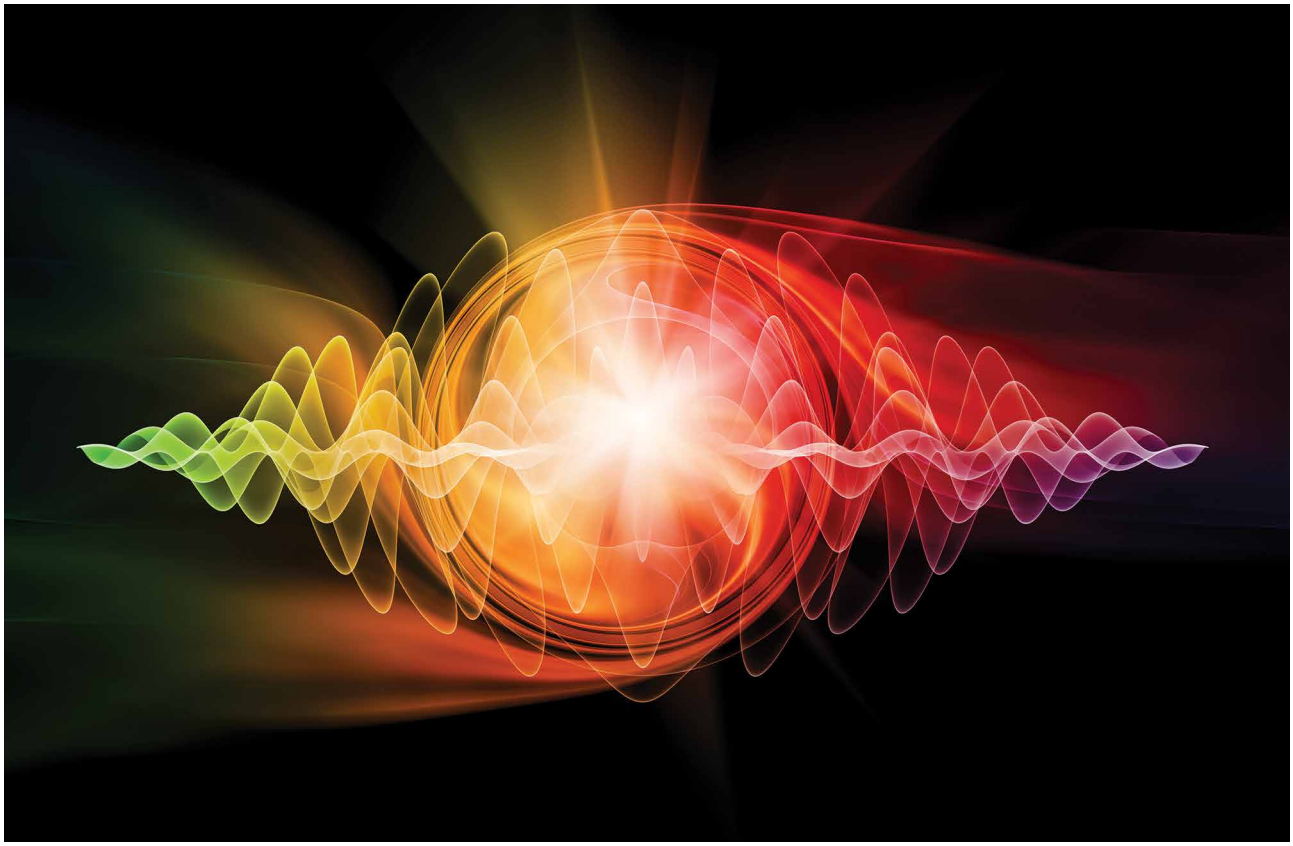
Computational chemistry is now routinely used for drug design, spectroscopy and solar energy devices, in addition to countless other applications. Through such calculations, it is possible to work out whether a particular reaction is chemically feasible, or how a molecule will interact with light, investigating whether or not it will make a good candidate for use in solar cells. However, the key problem in the field of computational modelling is that it is challenging to create models that are truly 'chemically accurate' – not only reproducing what has been experimentally observed, but also being reliable when used on systems where such experimental data is unavailable.

Improving the accuracy and versatility of computational models is one of the current challenges that Dr Kirk Peterson and his team at Washington State University are currently addressing. 'We aim for an accuracy that is useful to researchers carrying out sophisticated experiments, or even to supplant experiment in those cases were the experiments are too difficult or dangerous,' says Dr Peterson.

Constructing a Model

Atoms are made up of protons, neutrons and electrons. However, for the goal of calculating the chemistry of elements throughout the Periodic Table, it is the behaviour and the organisation of only the electrons that govern the majority of their properties related to chemical reactivity. Due to the small size of electrons, they need to be modelled using quantum mechanics and in particular, with the Schrödinger equation. This equation offers a means of describing the electrons in terms of an associated 'wavefunction' – or its wave-like character – which is the necessary ingredient

‘We use the methods of quantum mechanics to predict and interpret fundamental properties of molecules, such as their geometric structures and internal motions such as vibrations, as well as the energetics of the chemical reactions they may be involved in.’



for calculating experimental observables such as thermodynamic or spectroscopic properties.

Unfortunately, the Schrödinger equation can only be solved perfectly for a system with one electron – that is, the hydrogen atom – so for calculations involving larger atoms, or even molecules, approximate solutions are required. Finding methods to generate approximate but accurate descriptions of molecules remains a big challenge, and this is why the work of Dr Peterson and his team is so important.

Accurate Approximations

Dr Peterson and his group specialise in the development of ‘basis sets’. A basis set is a mathematical description of the electrons in an atom or molecule (or, more specifically, the wavefunction), which can be used in conjunction with a particular computational method of solving the Schrödinger equation to calculate various molecular properties, such as the strength of a chemical bond.

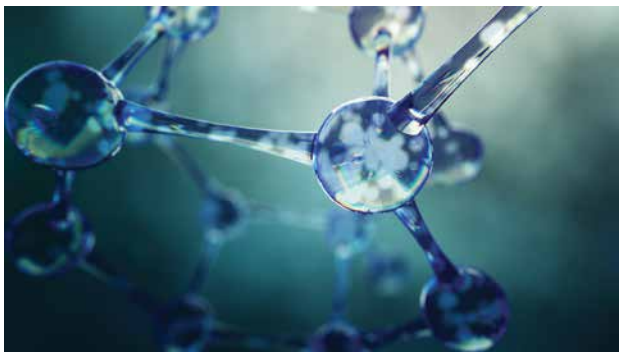
Each basis set is made up of a collection of different ‘basis functions’ – each contributing to a specific property of the atom or molecule. The challenge with designing basis sets is knowing what kind of these basis functions to use, and how many of them need to be used, to describe the properties of the atom or molecule accurately. An ideal set of mathematical functions would account for the behaviour of the negatively charged electrons due to the influence of the positively charged nuclei across a full range of electron-nucleus distances. The basis set also needs to be computationally tractable so that it is possible to compute properties of interest on reasonable timescales.

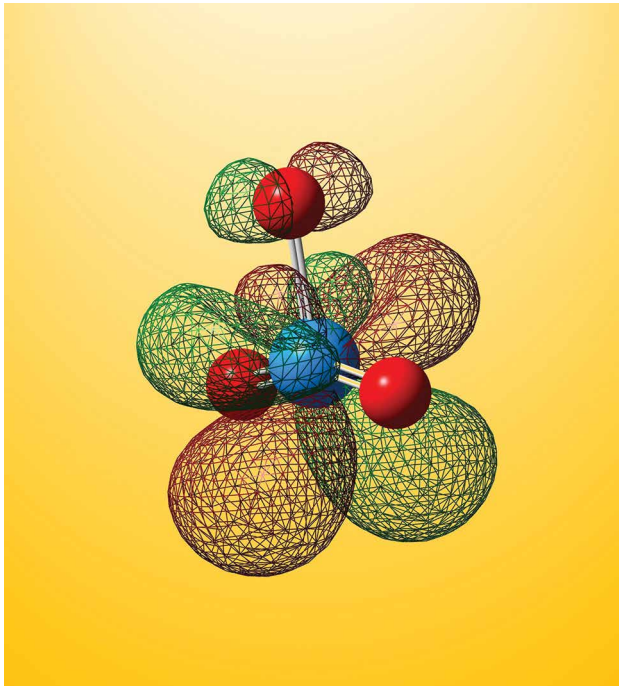
The most commonly used approach is to describe each electron’s wavefunction using Gaussian functions, creating a Gaussian-type basis set, which Dr Peterson is an expert in. In the simplest description of a molecule, a single basis function is used for each electron or electron pair in the system. When calculating molecular properties, such as the geometrical arrangement of the atoms in the molecule, each basis function adds a certain amount of time to the calculation, so the more electrons a system has the heavier the computational cost.

The problem is that Gaussian functions do not perfectly describe the physics of the electrons in the system, and so-called ‘minimal’ basis sets, where each electron has one associated basis function, reproduce experimentally-observed chemistry very poorly. This is obviously highly undesirable for scientists such as Dr Peterson and his colleagues, who are looking to produce highly accurate chemical models that can be considered sufficiently reliable, even in the absence of experimental results.

Bigger Is Not Always Better

While minimal basis sets generally do a poor job of describing chemical properties, the basis sets designed by Dr Peterson and others have several tricks to significantly increase the accuracy of the calculations performed with Gaussian functions. One approach is, rather than using a single basis function to describe each electron, multiple





functions can be used instead. Scaling and adjustments can be applied to each Gaussian function to better model the behaviour of specific types of electrons, for example, electrons that are not very tightly bound to the nucleus. Different angular factors are also applied to these Gaussian functions in order to describe the varying shapes of orbitals in the atomic or molecular wavefunction.

While the temptation may be just to include large numbers of basis functions to improve the accuracy of the computational model, things are not so straightforward in reality. For systems with large numbers of electrons, like the heavy elements Dr Peterson is interested in, using large numbers of basis functions for each electron means the calculations would take too long. This means that to design efficient basis sets to treat the lanthanides and actinides – the heaviest elements that possess between 57 and 103 electrons, and occupy the bottom two rows of the Periodic Table – the electrons need to be categorised further. Here, a distinction can be made between the outer electrons, which are actually important for chemical processes and the so-called core electrons, which, being closer to the heavily charged nucleus, are only spectators in most chemical processes so do not need to be treated with the same level of accuracy.

In particular, Dr Peterson's team's approach involves developing and using a sequence of basis sets of increasing size, such that they systematically approach the limit of an infinite set. At this 'complete basis set limit', usually obtained by extrapolation, the resulting accuracy of approximate solutions of the Schrödinger equation can be more easily assessed, much like an experimentalist attempts to understand all the sources of uncertainty in their experiments.

Dr Peterson and his team have designed many basis sets that are specifically to be used on these heavy elements – in order to calculate chemical properties with high accuracy. These basis sets are now used worldwide by other scientists who are looking for ways to understand the chemistry of this unique region of the Periodic Table.

Challenges Associated with Heavy Elements

Finding ways to reduce the number of basis functions while retaining the accuracy of calculations is not the only challenge scientists come across when dealing with the heaviest of elements. For these elements, the greater number of protons in the nucleus mean there is a sufficiently large density of positive charges for the electrons to experience 'relativistic effects', where their speed is sufficiently large that they become heavier, causing them to move closer to the nucleus. For the actinide elements, these relativistic effects are incredibly important, as the contraction of the innermost electrons can significantly change the strength of the interaction between the nucleus and electrons that are further away. Therefore, this can qualitatively affect the types of bonds and chemical compounds that can be formed compared to lighter elements.

Being able to model the chemistry of the actinide elements accurately is incredibly important, as experimentally creating and studying many of these complexes is very challenging. Many of them may only exist for very short periods of time and often under extreme conditions, such as very high temperatures. The computational cost and experimental challenges therefore mean that there are relatively few studies on the behaviour of these heavy elements.

Dr Peterson and his group are very interested in developing a more complete understanding of the trends in the Periodic Table. Elements in the same group, which appear in the same column of the Periodic Table, often have similarities in their chemical behaviour. By developing basis sets that are both computationally efficient enough to be used on large actinide systems, while including a description of the relativistic effects and other important physical phenomena, Dr Peterson and his group are now able to very accurately predict which actinide molecules are likely to form and which are not from their chemical properties.

Probing New Physics

Already, Dr Peterson and his team have been able to use these basis sets in conjunction with computational methods to describe the spectroscopy and chemical properties of many of the heaviest elements in the Periodic Table, with an unparalleled level of accuracy. 'Over the last few years we have focused on the early actinide elements, for example, thorium and uranium,' says Dr Peterson, and the basis sets that his team has developed can be widely used as general tools for the international computational chemistry community. Future work will involve refining the efficiency and accuracy of such basis sets, and the continuing increase in available computational power will make it possible to attempt even more ambitious calculations on the most interesting of chemical species. 'We are now turning our attention to molecules containing heavier elements like plutonium (Pu), curium (Cm), and even to more exotic elements like californium (Cf) and lawrencium (Lr).'

Meet the researcher

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Dr Kirk Peterson received his PhD in Physical Chemistry from the University of Wisconsin-Madison in 1990, where his thesis research involved both experimental spectroscopy and quantum chemistry calculations. He subsequently carried out postdoctoral research at the Universität Bielefeld, Germany and then the Pacific Northwest National Laboratory (PNNL) in Richland. He joined the Washington State University faculty as an Assistant Professor of Chemistry in 1994 and held a joint appointment in the Environmental Molecular Sciences Laboratory located at PNNL until 2002. He has been at the Pullman campus of Washington State University since 2002 and was promoted to full Professor in 2004. He currently holds the position as a Edward R. Meyer Distinguished Professor of Chemistry.

Dr Peterson is one of the world's leading researchers in the development of Gaussian basis sets for molecular calculations, as well as the accurate *ab initio* calculation of potential energy surfaces for applications in thermochemistry and spectroscopy. He has over 250 scholarly publications, including 16 book chapters and one textbook on quantum chemistry. Over the course of his career, he has achieved many awards, including the Washington State University College of Sciences Distinguished Faculty award and the Excellence in Graduate Teaching Award from the College of Arts and Sciences at Washington State University. He has been elected a Fellow of the American Physical Society, the American Chemical Society, and the American Association for the Advancement of Science.

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FUNDING

Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences of the U.S. Department of Energy (Heavy Element Chemistry Program)

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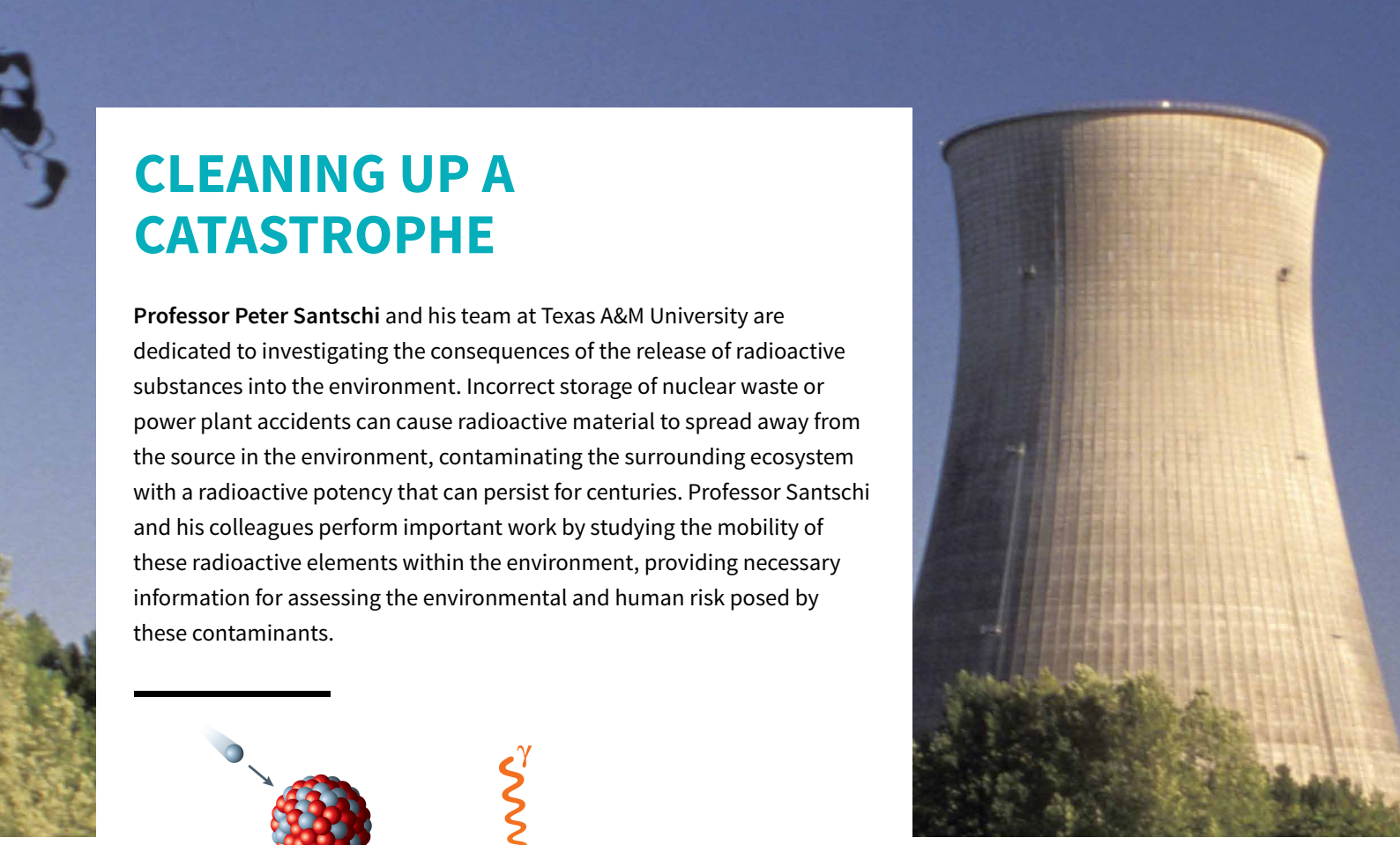
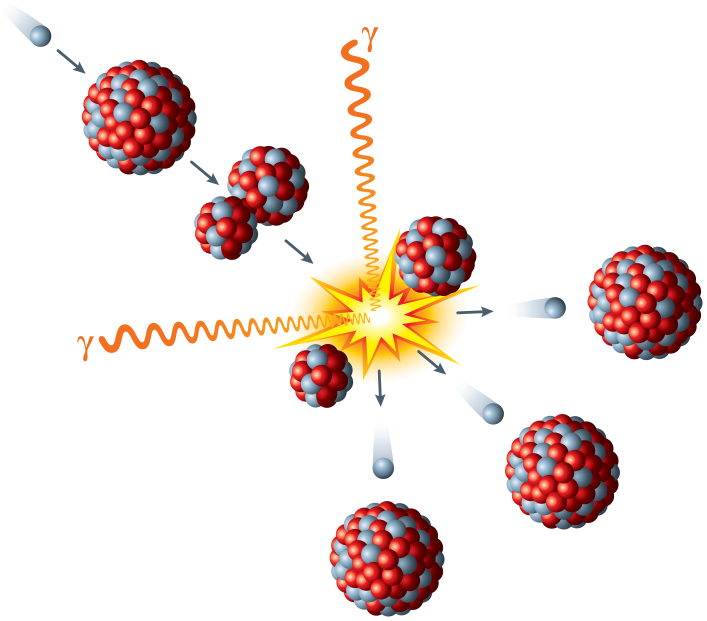
WASHINGTON STATE UNIVERSITY

CLEANING UP A CATASTROPHE

Professor Peter Santschi and his team at Texas A&M University are dedicated to investigating the consequences of the release of radioactive substances into the environment. Incorrect storage of nuclear waste or power plant accidents can cause radioactive material to spread away from the source in the environment, contaminating the surrounding ecosystem with a radioactive potency that can persist for centuries. Professor Santschi and his colleagues perform important work by studying the mobility of these radioactive elements within the environment, providing necessary information for assessing the environmental and human risk posed by these contaminants.





Recently, power generated from nuclear energy has undergone something of a renaissance due to growing concerns about greenhouse gas emissions. Countries such as India and China have pledged to build dozens more nuclear power plants in the upcoming decade. It's easy to see why, when you consider that a single gram of uranium-235 releases almost 300,000 times the energy of an equivalent coal source, with the added benefit of producing negligible amounts of greenhouse gas emissions. Whilst a fuel like uranium-235 isn't technically classified as a renewable energy source, it has been predicted that with future advances in reactor efficiency, especially with regards to recycling the waste, current reserves could potentially power the entire globe for 100,000 years.

Fundamentally, a nuclear reactor works by bombarding a heavy, radioactive atom such as uranium with neutrons in order to make it more unstable. This instability causes the radioactive nucleus to split into smaller atoms, emitting further neutrons in the process. This then sets off a chain reaction of uranium-235 atoms being split, and dividing it into smaller more stable atoms. Known as nuclear fission, this process produces an enormous amount of energy in the form of heat, which is then utilised to drive steam turbines in order to generate electricity with a high degree of efficiency.

While there are many advantages, working with nuclear energy is well-known for being a double-edged sword. The waste produced in the nuclear fission chain reaction is a major drawback of this power source. If not handled correctly, nuclear waste can be incredibly harmful to humans, and if released into the environment, it can have devastating consequences to any surrounding plant and animal life. It therefore has to be stored responsibly, with every effort made to ensure that there are minimal leakages for thousands of years. However, despite all the precautions taken, leakages of radioactive waste into the environment have happened multiple times throughout history.

Just Another Day at the Office

Professor Santschi and his team carry out their work at some of the world's most irradiated areas. Most of these sites became contaminated over 50 years ago, with the initial discovery of nuclear reactions, and the production of nuclear weapons and their testing. This sparked the arms race and the Cold War. In the past, less was known about the immense dangers of nuclear waste, or the contamination in the surrounding environments at some of these production sites. Two of these facilities, where Professor Santschi and colleagues conduct their research, are the Savannah River Site in South Carolina and the Hanford Site in Washington State. These sites were formally used by the Department of Energy to make nuclear materials for defence purposes, as opposed to energy purposes.

This leaked radioactive waste has the potential to then spread throughout the environment in a number of ways. As an example, rainwater can wash the radionuclides (radioactive atoms) down through the soil and into the underlying aquifer where it can be transported to any number of aquatic environments. At the Hanford Site alone, there are hundreds of acres of surface aquifer contaminated with radioactivity that are presently undergoing remediation.

Professor Santschi and his team also study samples from the site of the infamous Fukushima Daiichi Nuclear Power Plant in Japan. When in 2011, an earthquake-induced tsunami struck the plant, the wave's impact destroyed its power source and backup generators. The reactor units were then improperly cooled down and the reactor core went into meltdown. This catastrophe caused the release of massive amounts of radioactive substances into the surrounding atmosphere and into the Pacific Ocean. Thankfully, disasters like this are uncommon, but when they do occur, the sheer volume of radioactive material released can have a devastating impact on the surrounding environment.

Releasing Radioiodine

A common waste product of the nuclear fission reaction are two forms of radioactive iodine, known as iodine-129 and iodine-131. With a difference of only two neutrons, iodine-129 and iodine-131 have radically different properties. The isotope iodine-131 is produced much more readily in fission reactions, but is much more short-lived, with a half-life of only eight days. This means that for a given sample of iodine-131, half of the atoms in the sample will have decomposed into non-radioactive atoms after just 8 days. In contrast, iodine-129 is less common in nuclear fallout, but as a beta emitter with a half-life of 16 million years, measuring it is more challenging. While these forms of radioiodine occur naturally in tiny quantities, the majority present in the world comes from human activity, due to accidental leakage or nuclear disasters.

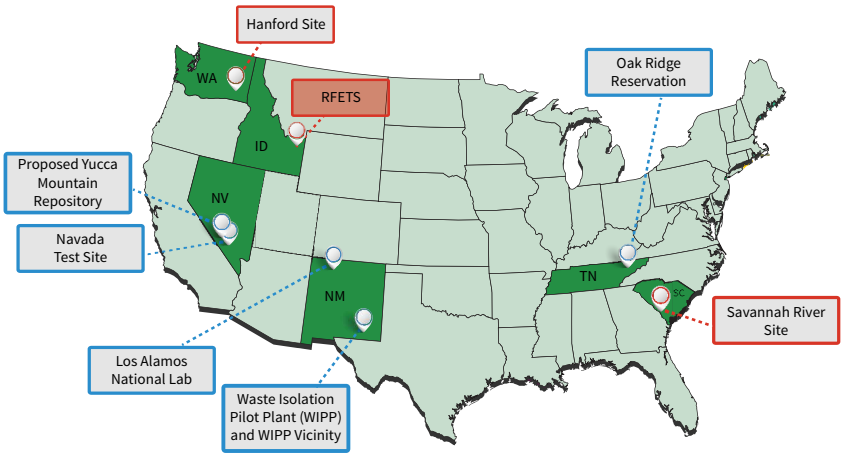
Iodine is required by the human body, with almost all of it being stored in the thyroid gland, where hormones for controlling growth and metabolism are produced. If the body were to be exposed to large amounts of radioiodine, it would be collected and stored here in the same way. This has been the case for workers of the Chernobyl and Fukushima power plants, where a nuclear disaster exposed them to massive amounts of radioactive particles. Tragically, the radioiodine that was absorbed and concentrated in their thyroid, bombarded the surrounding tissue with high doses of radiation, has the potential of leading to cancer.

Although all forms of radioiodine are dangerous, the dangers of iodine-131 are not as stark as those of iodine-129. Because of its short lifetime, iodine-131 doesn't pose as significant a threat to humans and the environment. Ironically, it can actually be used to treat thyroid cancers, as it releases radiation that can kill cancer cells, and then swiftly decays into the stable and harmless element xenon-131. Iodine-129 is much more problematic because of its long-lasting potency, and its tendency to bond with other molecules.

Ground-Breaking Research

Professor Santschi and his team have been studying the effects of this radioiodine interacting with the environment for over 10 years. He realised that when radioiodine or any other radionuclide is released, reactions will occur between these hazardous substances and the neighbouring natural organic matter. Professor Santschi explains that his research 'asks the question: what organic molecules carry radionuclides in the environment?' He goes on to say that 'answering this question requires one to bridge the gap between environmental radiochemistry and environmental organic chemistry, which normally are two separate scientific disciplines with each asking their own questions, and requiring very different training and knowledge.'

Radionuclides that are exposed to the environment go through several complicated reactions with surrounding matter. When exposed to aquatic environments, radioiodine can exist in multiple chemical forms (oxidation states) and can bind strongly to natural organic matter, making environmental remediation challenging. Standard models for predicting how nuclear waste propagates through the environment often assume that radionuclides remain in the same oxidation state and fail to take into account interactions with natural organic matter.



USA nuclear waste sites

Professor Santschi and his colleagues developed a brand-new approach to determine the amount of iodine present in the environment. They used a technique known as Gas Chromatography/Mass Spectrometry (GC-MS), as well as Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR-MS) and Nuclear Magnetic Resonance (NMR) at their collaborator's facilities, to give much more detailed insight into what forms of iodine were present in the soil. Previous techniques could only measure iodine at very high concentrations that would never be found naturally, so the real breakthrough of this technique is that it allows the various iodine species, and isotopes, to be detected at concentrations that are environmentally relevant.

Complex Reactions

When iodine-129 is created as a by-product of nuclear power and released to the environment, it can become negatively charged by accommodating an extra electron. This form of iodine ion is known as 'iodide', and most conventional models only account for this form when attempting to calculate the dispersion of radioiodine. As iodine can exist in seven different oxidation states, Professor Santschi and his team realised that the reality is much more complicated. These differently charged iodine ions behave in completely different ways and will either flow more easily or less easily into the environment depending on the state.

There are many ways in which radioiodine can be altered when exposed to the environment. If the extra electron of iodide becomes lost to a surrounding substance, another iodide will be able to bond with it to produce the diatomic molecule I_2. I_2 is how elemental iodine exists under standard room temperature and pressure conditions; however, the bond is not particularly strong, so further reactions can occur if I_2 is in the presence of oxygen. Most commonly, a threefold negatively charged species, IO_3^-, called 'iodate' is expected to form. Radioiodine can also bind in numerous ways to the carbon in natural organic matter. All of these reactions make radioactive iodine more likely to bond to natural organic matter compounds, creating stable organic iodine molecules. The group found clear evidence that this organo-iodine formation is mediated by enzymatic reactions and microbial activity. The stability of all of these molecules changes the way the iodine would usually propagate, making it more difficult to extract and clean up.

Professor Santschi's group also found clear evidence that another radionuclide, plutonium – also a potentially toxic radionuclide – is strongly bound to specific natural organic matter compounds in surface soils. However, unlike iodine, which is directly bound to aromatic compounds similar to how it occurs in our body, plutonium was found in the company of strongly iron-binding compounds called 'hydroxamate siderophores' in chemically separated plutonium enriched fractions. Hydroxamate siderophores are among the strongest binding agents for plutonium, with some of them binding even stronger to plutonium than to iron. These compounds are naturally produced to mobilise iron from soils to make iron (which is normally insoluble) available to microorganisms and plants. However, these compounds were unequivocally found in the macromolecular and particulate fraction. The team concluded that it is highly likely that plutonium is bound to those siderophores, catching a ride on the 'iron wheel'.

For both elements (iodine and plutonium), their strong binding to naturally produced organic macromolecules under environmentally relevant concentrations has shown unexpected behaviour with respect to their mobilisation and immobilisation potential. Professor Santschi's group's low-level approach simulating ambient behaviour is complementary to synchrotron radiation techniques that are commonly applied by radiochemists – approaches that work only at higher concentrations. However, the team showed the importance of working at ambient environmental concentrations, where their behaviour can be different from that expected at higher concentrations.

Environmental Impact

The significance of studying these less-mobile radionuclide-containing molecules is that they can potentially pose a much greater health risk to humans. The standard form of radioactive iodide, for example, can spread easily throughout the environment, making it more diluted and less of a significant health risk. However, the forms of iodine that are more likely to remain in soil pose different risks. While it is beneficial that these forms are less mobile, and therefore can be monitored more effectively and potentially recovered, less mobile molecules remain in the soil for a significant amount of time, and may be taken up by plant matter and incorporated into their structure. Once taken up by plants, herbivorous livestock can consume this radioactive fodder, converting it into muscle tissue, which would be carcinogenic to humans if eaten as meat. Alternatively, radioiodine that reacts in aquatic environments can be taken up by fish in a similar way, which would then become equally harmful if consumed.

The importance of this work can have impacts in all areas of the environment. Professor Santschi explains that principle of these techniques could help not only environmental remediation of existing contaminated sites, but also provide information that can be used to estimate risk posed by accidental release, such as Fukushima, and thus create information that is being used to minimise risk posed by long term disposal of waste.

Meet the researcher

Professor Peter H. Santschi
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Professor Peter Santschi obtained his PhD in Chemistry in 1975 from the University of Bern in Switzerland. Since then, he has worked as a researcher at various prestigious institutions, such as Columbia University, the Swiss Institute for Water Resources and Water Pollution Control and the National Taiwan University, to name just a few. Professor Santschi is currently a Professor in the Department of Marine Sciences at Texas A&M University. His research interests include a broad range of topics in Marine and Environmental Chemistry, including the role of natural nanoparticles in the biogeochemical cycling of trace substances, tracer applications using radioactive and stable isotopes, relationships between trace elements and natural organic matter, and the importance of exopolymeric substances for trace element binding and removal from natural waters. Over the course of his career, Professor Santschi has been the recipient of many awards and honours, including the Distinguished Achievement Awards in Research, as well as Graduate Student Mentoring from Texas A&M, and he is an elected Geochemical Fellow of the Geochemical Society, the European Association of Geochemistry and Fellow of the American Geophysical Union.

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FUNDING

Department of Energy, Office of Science, Subsurface Biogeochemistry Research (SBR) program
National Science Foundation, Division of Ocean Sciences, Chemical Oceanography Program

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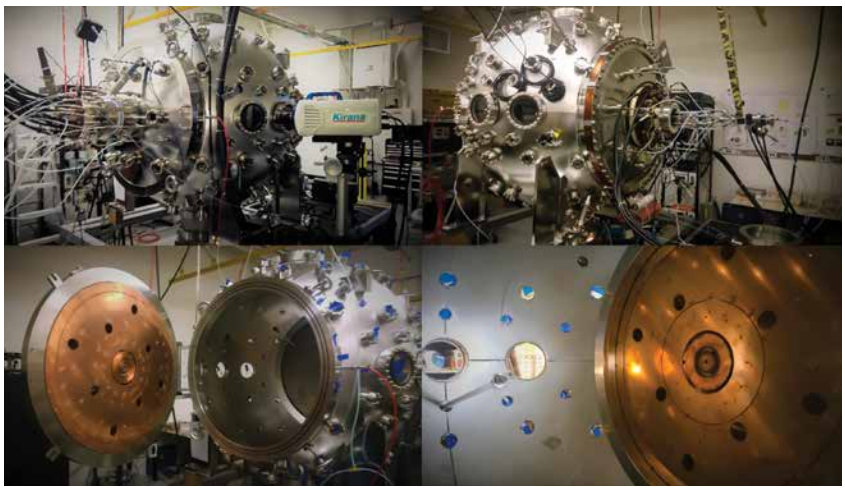
TEXAS A&M UNIVERSITY

HOPE FOR HUMANITY IN THE ENERGY CRISIS: ASTRONOMICAL JETS IN A LAB

If we consider Earth as a closed box in which humanity has only ever lived, the second law of thermodynamics says that in the end, inevitably, the box will reach a state of maximum disorder. So, in the long run, there are two important ways in which our species might cope with the issue: switch to increasingly cleaner energy sources to push the deadline further away, and colonise the solar system to expand the size of the box. **Professor Setthivoine You** and his team at the University of Washington are currently working on making both outcomes possible.

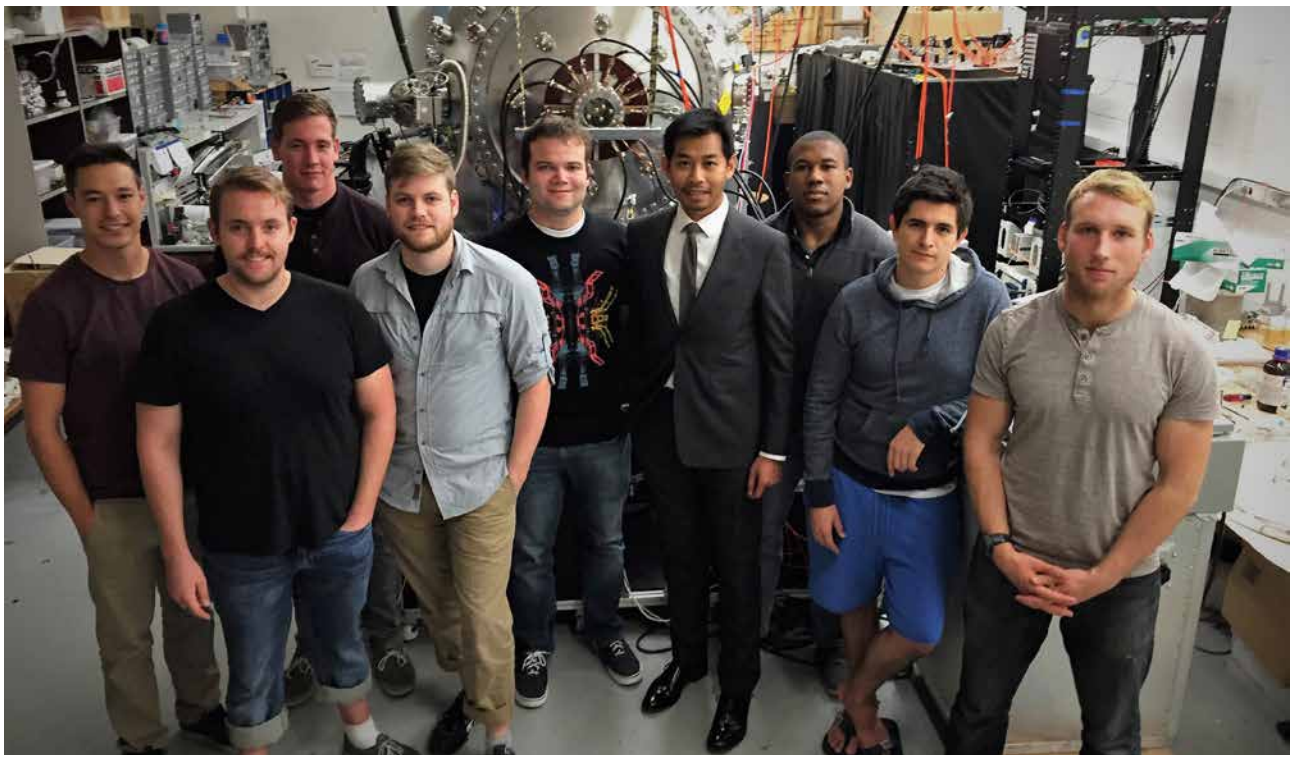


The long road of civilisation has progressed with our ability to harness various forms of energy for power and transport. In the first age, fire was used for warmth and to light our way, while our feet carried us. Next, wind filled our sails, and we used animals to transport our goods and ourselves. In the third age, fossil fuels gave rise to an industrial revolution that has powered our modern civilization. Through the ages, the energy humans have harnessed has ultimately come from the Sun, which has been stored chemically and thermally – wood stores the energy of solar rays, animals feed on plants, wind blows due to uneven warming by the Sun, and fossil fuels that have stored the Sun's energy from eons before.

The fourth age began with the scientific discovery of subatomic particles. One important implication of this was the development of nuclear energy. Within this nuclear age, we have left the Earth to explore our solar system, observed our planet from above, and built an internet that connects us and gives us unlimited access to information. All of these achievements, all those before and all those to come, rely on a continuous supply of energy and raw materials. Unfortunately, however, harnessing energy causes pollution and climate change, while digging for raw materials wrecks the ground. What if we could have a technology that could solve these problems? The ideal long-term solution would be to have a clean energy source that is not dependent on limited fuel supplies, and to then use this energy to colonise the solar system for raw materials instead of excavating our Earth. This technology has actually been pursued for decades – a technology that not only could eliminate the largest ecological crisis our species has ever encountered, but one that could spur a migration unlike any ever seen before. That technology is nuclear fusion, and it's the same process that fuels the Sun.

Going Nuclear: Fusion vs Fission

Nuclear energy isn't a new phenomenon – we've had nuclear fission working for decades – but the subtle differences between fusion and fission have a substantial impact on power output. Nuclear fission is the splitting of heavy atoms into two fragments, achieved by bombarding them with neutrons (a type of uncharged subatomic particle). The process takes heavy elements like plutonium or uranium and splits them into lighter elements such as barium and lanthanum. During this reaction, a tremendous amount of energy is released – and it can be transformed into electrical power by heating water to produce steam to turn turbines. This is the same method used for practically all of our electricity generation, basically by replacing the coal or natural gas furnace with a fission reaction chamber. The advantage is that fission releases six million times more energy per kilogram of fuel than fossil fuel combustion. Therefore, instead of consuming 3 million tonnes of coal per year which releases 60 thousand tonnes of carbon dioxide (the key driver behind climate change) into the atmosphere, a typical power plant would only consume 250 tonnes of uranium, which releases no carbon dioxide, but produces 60 tonnes of dangerous radioactive waste.



Nuclear fusion, on the other hand, aims to do the opposite – it takes very light elements such as hydrogen and transforms them into heavier elements such as helium, by subjecting them to extremely high temperatures and pressures in an attempt to mimic the conditions at the centre of stars, such as the Sun. The advantage is that fusion produces four times more energy than fission per kilogram of fuel, so even less fuel would be needed. No direct radioactive waste or carbon dioxide is produced, only benign helium, and the reserves of hydrogen isotopes in the oceans are sufficient to last for hundreds of thousands of years.

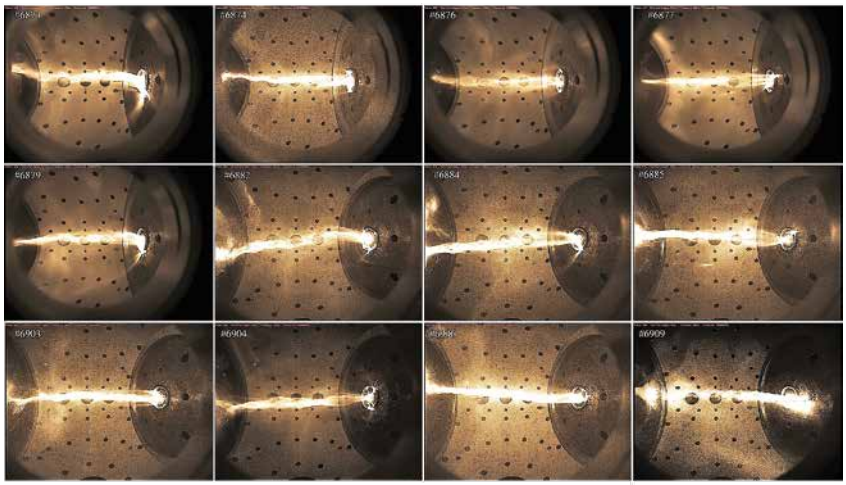
However, contrary to fission or fossil fuels, the nuclear fusion process requires a vast amount of energy to get going. This can be likened to the process of lighting a match, where we need to put sufficient kinetic energy into the system by striking the match vigorously enough to heat the matchhead until it begins burning on its own. If we don't strike it sufficiently, it only heats the matchhead. In fusion energy research, decades of scientific experiments have been striking this match with bigger and bigger machines. From small university-size experiments in the 1950s to the largest experiments in Europe, Japan and the US today, we have reached the point of breakeven (when the fusion energy output equals the heating energy input).

With the world's largest fusion experiment – the pharaonic international ITER project – currently under construction, we are now moving towards the point of ignition (when the fusion energy output can sustain itself). But to be competitive, fusion energy must ultimately find a way to reduce the size and complexity of the reactors. Therefore, scientific research into the fundamental processes inside fusion systems, to understand the delicate interplay of turbulence, plasma flows, and magnetic fields, promises to make fusion energy reactors small enough to put on spacecraft. Professor Setthivoine You and his team at the University of Washington are one such team of scientists working towards obtaining this feat.

For the fusion process to work – that is, to get more energy out than you put in – three conditions must be fulfilled simultaneously: the fuel must be heated to more than one hundred million degrees, there must be sufficient fuel density, and the whole system must be confined together sufficiently long enough. Above 11,000°C, the fuel exists in the form of plasma – one of the fundamental states of matter (along with solid, liquid and gas). Plasma is effectively a gas that has been super-heated until its atoms begin to lose their electrons. The resulting matter contains negatively-charged free electrons and positively-charged ions. Plasmas are interesting because, unlike the other states of matter, the charged particles within plasma react strongly to magnetic fields. We can therefore use magnetic fields to keep hot plasma away from cold walls, and we can shape plasmas out the back of thrusters to propel spacecraft. But plasmas also exist naturally.

Here on Earth, plasmas exist naturally in lightning but are mostly created artificially – in plasma TVs, fluorescent lighting and ion thrusters designed for electric space propulsion. In space, however, you can find plasma occurring naturally in the magnetosphere, in the solar corona and the solar wind, in the cosmic interstellar medium, at the centre of stars, and in astrophysical jets. In fact, over 99% of matter in the visible universe is believed to be in the form of plasma.

Astrophysical jets are a particularly fascinating astronomical feature as they extend out for light years from the centre of accretion disks (disks of matter rotating around a central body, such as a star or black hole) in remarkably collimated beams. The exact mechanism that causes this is unknown, yet it is clear that strong plasma flows interacting with magnetic fields play a crucial role. Understanding how astrophysical jets are so long, so straight, and so stable can help us understand how to make fusion plasmas more stable, more compact and remain confined for longer. Astrophysical jets are natural nozzles, and understanding them can help scientists to improve plasma thrusters for electric space



propulsion. This is just one aspect of a project that Professor You and his research team are working on.

The Mochi.Labjet Project

The Mochi.Labjet project is essentially a laboratory-based astrophysical jet created by Professor You and his team to study canonical flux tubes (tubes of magnetic plasma) and plasma self-organisation (the tendency of plasma to organise itself into complex arrangements on its own). As Professor You describes: 'The Mochi project is a theoretical and experimental program designed to study the fundamental physics of plasma self-organisation. The goal is to understand and eventually harness this remarkable property of plasmas for compact magnetic fusion, understanding natural plasmas such as astrophysical jets and improving plasma space propulsion with magnetic nozzles.' He goes on to say that, 'the experiment replaces an accretion disk, that would rotate in a vacuum chamber at impractical speeds, with three independent concentric annular electrodes.'

The electrodes are used to mimic the rotation of an accretion disk around celestial objects, and this novel approach allows Professor You and his team to simulate and study astrophysical jets with reproducible and carefully-controlled experimental conditions. This up-close and personal manner of studying jets complements astronomical observations that are restricted to single viewpoints in space and time. The team's aim is to verify predictions by the theory of canonical flux tubes that magnetic fields can be stabilised by helical flows, which can then be used in a variety of different applications, from nuclear energy to space travel. 'With this theory of canonical flux tubes and the well-diagnosed experiment, the research program intends to improve the theoretical understanding of how astrophysical jets are highly collimated, often very straight and extremely long,' says Professor You.

As mentioned above, plasmas can self-organise: they have a natural tendency to re-arrange themselves into various shapes on their own. Some of the shapes are like astrophysical jets launched from accretion disks, others are like donuts used in attempts to achieve fusion energy, while some are like arches that protrude from the surface of the Sun. The transition from one shape to another often involves flows, heating, and re-shaping of magnetic fields. These shape transitions can involve large instabilities, while at other times it stabilises them. Exploiting these spontaneous processes could help make magnetic donuts more stable and more compact by converting magnetic energy into flows, therefore helping to make fusion reactors smaller and cheaper. 'Beyond laboratory astrophysics, the experiment can form plasma configurations to study the interaction between flows and magnetic fields,' explains Professor You. 'For example, in donut-shaped configurations suitable for fusion energy, flows can improve confinement and reduce the size of future reactors.' As current technologies result in fusion reactors that are on the same scale as football stadiums, Professor You's research has the potential to change the field of nuclear energy.

Aiming for the Stars

Along with playing a part in providing humanity with a potentially limitless energy source, Professor You's research could also help usher in a new age of space exploration based on plasma engine technologies. Space travel involves converting energy stored in some form of fuel into kinetic energy to cover the vast distances in the cosmos. Nuclear fusion therefore has the potential to open up the solar system to human colonisation. But before this futuristic technology is achievable, plasma thrusters based on solar electric power already propel spacecraft around Earth and into deep space. They convert solar power into electrical power, which is then used to generate plasma. Then, using electric or magnetic fields, the plasma is ejected out of the rear of the spacecraft as an exhaust plume with much higher speeds than has ever been possible with chemical fuels. In space, higher exhaust speeds mean that you can use less fuel to go further and faster.

Plasma engines are the key to interplanetary travel, with NASA and private companies recently investing in plasma engines that promise to cut, for example, the journey time between Earth and Mars to just 39 days instead of 9 months. But going to Mars and beyond with heavy payloads such as human crews requires more energy than is available solely with solar power. Solar power coupled to plasma thrusters could be replaced by nuclear fission reactors coupled to the same plasma thrusters. But ultimately, fusion energy would be even more efficient, producing more thrust per kilogram of fuel directly from the plasma exhaust of fusion reactions. In this way, Professor You's work on plasma jet collimation and stability has the potential to do just that.

In the meantime, when asked about the future direction of his research, Professor You keeps his feet firmly planted on the ground: 'Another application is for space technologies such as plasma propulsion and space debris removal. A pair of plasma jets can control a target in space without any physical contact, so could de-spin and de-orbit debris to clean up the orbital environment. High power magnetised plasma jets could enable rapid interplanetary travel and the Mochi configuration has the advantage of a well collimated, high power plasma plume.'

There's a short phrase used in science to describe promising research with multiple applications – the sky is the limit. But if the intellectual investment of Professor You and his research team pays off, the sky won't be their limit – it will be their domain.

Meet the researcher

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Setthivoine You completed his MSc in physics at Imperial College, London in 1997, before going on to complete a PhD in plasma physics at the same institution in 2002. His research interests include plasma physics, laboratory astrophysics, magnetic flow measurement, fusion energy and space plasma propulsion. During his career do date, which has spanned four posts in three different continents, he has contributed to 22 journal publications, 54 conference proceedings, given 28 conference talks and attended 37 national and international conferences. He acts as a reviewer for numerous international journals and publishers and has been awarded multiple distinctions for his scientific work.

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FUNDING

US DOE
US DOE-SBIR
DOE-GSRP
UW AA

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MochiLabJet

LITERAL SUN JARS: SHRINKING STARS FOR ENERGY PRODUCTION

Science is the pursuit of knowledge – a search for an understanding. Sometimes that knowledge is simply collected and catalogued away for future reference (the laser was discovered in this manner) but, often, it is searched out vehemently to achieve something of importance. No other scientific endeavour has the potential to change the course of human history as much as Nuclear Fusion. And that's precisely what **Professor Michael Brown** and his team at Swarthmore College are working on.

If you've ever been in a supermarket during the summer months, you'll probably have come across a Sun jar. These small, solar-powered jars emit a steady glow of diffuse light and are so popular that a quick internet search returns countless do-it-yourself guides on how to make them for your garden. They look fantastic – almost magical – on a sultry summer's night, when the Sun has gone away but the temperature remains comfortable enough to stay outside and enjoy the evening, and when the barbecue has burned down to a scattering of glowing embers. In such a serene setting, you'd be forgiven for indulging in the belief that Sun jars might actually contain a tiny part of the Sun itself – an idea reminiscent of fairy-tales and folklore but, somewhat surprisingly, an idea that forms the basis of one of the most important scientific pursuits of the twentieth century: nuclear fusion.

The Search for an Eternal Energy Source

One of the greatest problems humanity is ever likely to encounter is human-induced climate change. While the mass media might have you believe that the subject is a controversial one, over 97% of practicing climate scientists agree that global warming is the result of human activities, such as burning fossil fuels to generate energy. In other words, we need to act now in order to avoid a climate catastrophe for ourselves and for future generations.

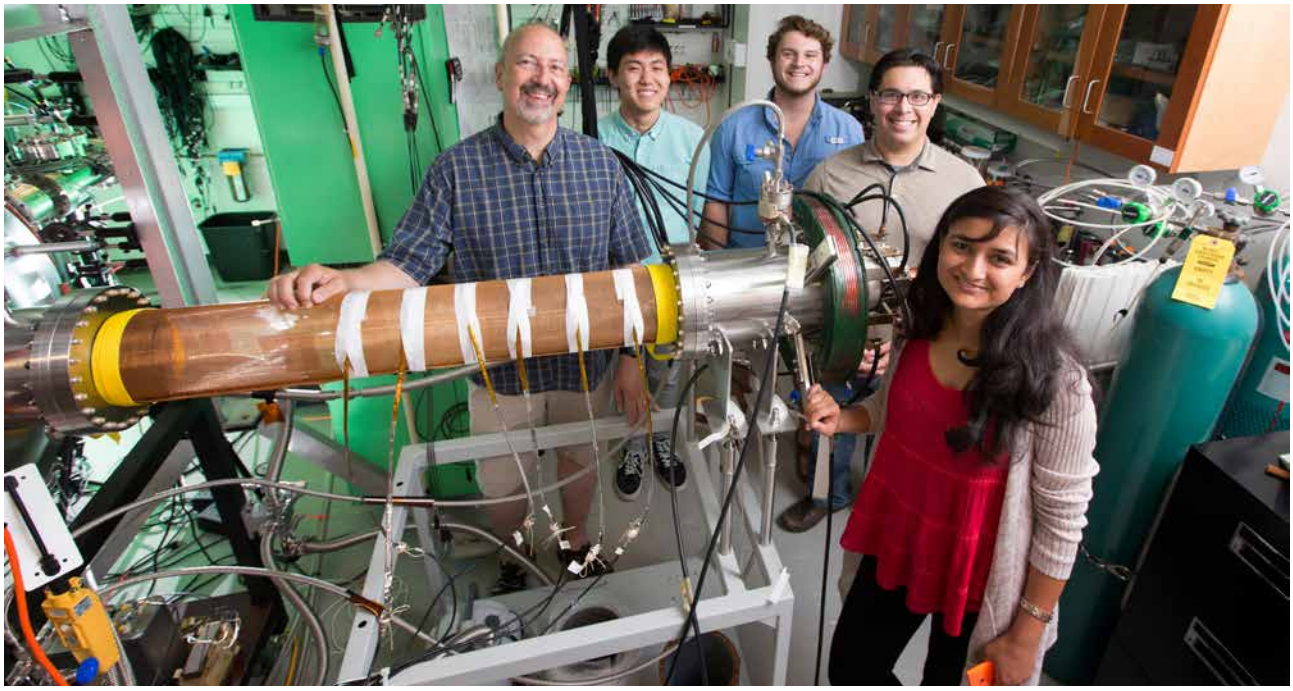
Virtually all of the energy that we rely on for fuel and electricity comes from the Sun. Plants feed on sunshine during photosynthesis, animals and sea creatures feed on these plants, and when living things die, they can become ultimately transformed into fossil fuels such as coal, oil and natural gas through a gradual process that takes millions of years. Burning these fossil fuels releases carbon dioxide into the atmosphere – the primary driver of global warming – and so we must drastically reduce our reliance on them if we are to prevent the most catastrophic consequences of climate change.

Most of our renewable energy can also be traced back to the Sun. Wind, for example, which turns turbines across the world day and night, is a result of inequalities in areas of atmospheric pressure caused, themselves, by differences in air temperature. Biomass – plant matter grown using sunlight – is either used directly as an energy source through combustion, or can be converted to biofuel through additional processes. Solar cells capture light emitted from the sun and convert its energy directly into electricity. But where does the Sun get its energy?

Nuclear Fusion

Stars, such as our Sun, begin their lives in stellar nurseries – extremely large clouds of gas and dust with a roughly continuous density (known to physicists and astronomers as a homogeneous state). However, due to the universal tendency for things to become less ordered as time progresses, some gas and dust particles inevitably bunch together causing localised areas of slightly higher density.

‘Attaining fusion on Earth requires achieving stellar densities and temperatures, and holding both for a substantial period of time’



As the strength of gravity depends on the amount of mass, and the mass of an object depends on its density, the gravity of such areas begins to attract more and more particles of gas and dust in a self-perpetuating process. Each particle drawn into our new ‘protostar’ causes the density at its centre to increase. As more and more particles arrive, the density – and temperature – becomes so great that the nuclei of hydrogen atoms can actually fuse together to form helium nuclei. This process – called ‘nuclear fusion’ – releases even more energy into the mix, which allows greater numbers of nuclei to fuse together, continuing the cycle. This self-perpetuating process is what will power the newly-formed star for the rest of its life.

While most of the energy we use can be traced back to nuclear fusion in the Sun, researchers such as Professor Michael Brown and his team at Swarthmore College, Pennsylvania, are trying to recreate this process here on Earth. As you might imagine, the problem is not a trivial one: ‘Attaining fusion on Earth requires achieving stellar densities and temperatures, and holding both for a substantial period of time,’ Professor Brown explains. Harnessing the process that the Sun uses to produce its energy has the potential to outshine all other sources of energy on Earth.

The ARPA ALPHA Project

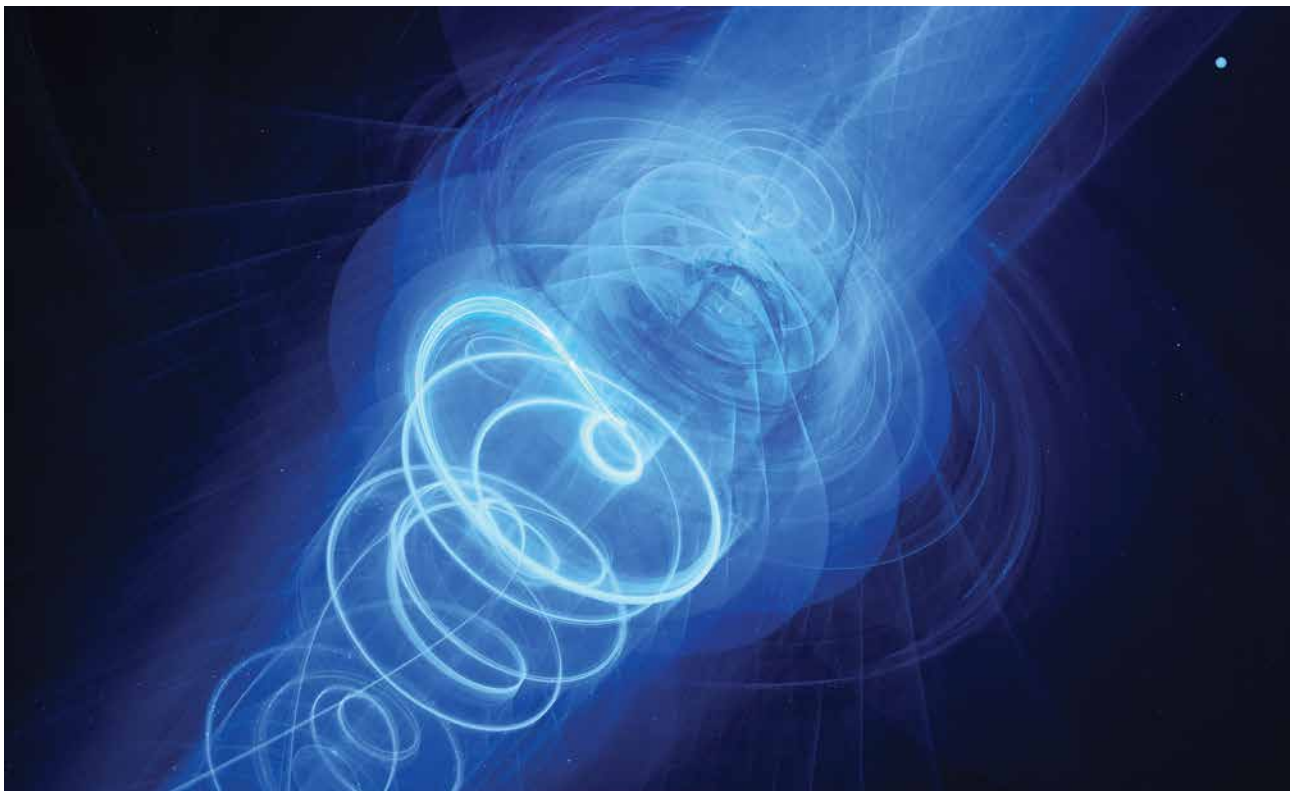
Nuclear Fusion has long been the pursuit of scientists around the world. It’s the holy grail – not only potent enough to satisfy all of society’s energy needs, but potentially capable of providing us with a means of exploring our galaxy (if you’re a fan of sci-fi, you will probably already be familiar with the concept of a ‘fusion drive’) – and pulls in billions of pounds of funding each year. Currently, there are two major players in this field: The National Ignition Facility (https://lasers.llnl.gov/), a $20 billion project near San Francisco that aims to use lasers to substitute the vast gravitational pull of the Sun – this is known as Inertial Confinement Fusion (ICF); and the ITER project in France (https://www.iter.org/), another $20 billion project that is hoping to produce fusion reactions in a process known as Magnetic Confinement Fusion (MCF). There are, however, smaller-scale projects taking place around the globe that hope to advance the field of Nuclear Fusion at a fraction of the cost.

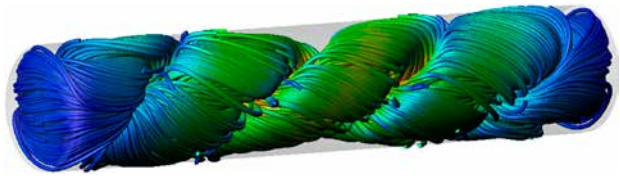
One such project is the Accelerating Low-Cost Plasma Heating and Assembly (ALPHA) scheme (https://arpa-e.energy.gov/?q=arpa-e-programs/alpha) funded by the US Department of Energy (DOE) through the Advanced Research Projects Agency – Energy (ARPA-E) branch. Professor Brown and his team work on a project known as the Swarthmore Spheromak Experiment (SSX, http://www.swarthmore.edu/ssx-lab), which is supported through the ARPA-E ALPHA project and aims to explore a process known as Magneto-Inertial Fusion. Magneto-Inertial Fusion, or ‘MIF’, is an intermediary approach, somewhere between ICF and MCF, which Professor Brown describes as ‘a new approach to fusion energy, to generate small parcels of hot magnetic plasma, then compress them, like when petrol is compressed in a car engine.’

‘Mainline fusion efforts cost several billion dollars,’ Professor Brown adds. ‘What we are working on is risky but potentially much cheaper.’ These small parcels of plasma essentially contain the same ingredients as the centres of stars but are on the same scale as the Sun jars mentioned earlier. To create these literal Sun jars, Professor Brown and his team of researchers are investigating the use of something they call a ‘Twisted Taylor State’ as the fusion medium.

The Twisted Taylor State

So, what exactly is a Twisted Taylor State? It’s essentially a volume of plasma – a hot gas of charged atoms – that is formed into a twisted structure using magnetic fields. ‘We first observed the structure at our lab in 2014,’ says Professor Brown. ‘Our experiments now concern measuring the Equation of State of





this parcel of plasma, so that we can predict how the temperature and density might change as we compress it.'

The Equation of State (EOS) is a mathematical relationship that describes how the pressure, temperature and volume of a gas – or plasma – interact with each other. Understanding the EOS of a system allows scientists to make accurate predictions about how that system will evolve over time or respond to external factors. 'Our goal for the ALPHA project is to accelerate a Taylor State to high speeds, then stagnate and compress the object into a suitable fusion target,' says Professor Brown. This will allow his research team to investigate if a Twisted Taylor State of plasma could be used to produce nuclear fusion reactions.

As you might expect, the SSX team employ a variety of complicated techniques and apparatus in their pursuit of nuclear fusion – coaxial plasma guns, stagnation flux conservers, ion Doppler spectroscopy and HeNe laser interferometry are just a handful of terms that feature throughout their publications. What you might not expect, however, is that the research team using these technologies primarily comprises undergraduate students. Swarthmore College is an example of a Liberal Arts College – of which there are hundreds in the US – where the focus is on undergraduate study within the fields of Liberal Arts and Science. In contrast to the UK, where research is primarily undertaken by postgraduate students and post-doctoral researchers, Professor Brown's team mainly consists of senior undergraduate students, including Emma Suen-Lewis, Luke Barbano, and Jaron Shrock who have each contributed substantially to the project'.

Progress so Far

Although the project is far from complete, Professor Brown and his team have already made some promising progress: 'We have completed analysis of compression events of our un-accelerated Taylor State and have identified a good model EOS,' he says. 'Results are being reported in two papers under review.' This model EOS will be used to guide their experiment when they begin to ramp up to more extreme states of compression that are more in tune with what's expected for the nuclear fusion process to start. 'When we push to more extreme compression, we will be guided by our EOS to predict densities, temperatures, and magnetic fields,' Professor Brown explains.

On the future of the project, Professor Brown is optimistic. He feels that his team is in a strong position to complete their work during the second half of the project: 'Our postdoc, Manjit Kaur, now has over a full year of experience, and we have assembled a team of talented collaborators including Swarthmore students, the simulation team, and Bryn Mawr Professor David Schaffner.' With the ability to satisfy society's energy needs through this new method of clean energy generation, it's no understatement to say that the work being undertaken by Professor Brown and his students has the potential to change the course of human history.

Meet the researcher

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Professor Michael Brown completed his undergraduate degree in physics at Pomona College in 1981, before obtaining a PhD from Dartmouth College in 1987. He lectured at the California Institute of Technology and Occidental College before moving to Swarthmore College in 1994, where he is the Morris L. Clothier Professor of Physics. His research interests include magnetothermodynamics, turbulence, fusion energy, and self-organisation in turbulent systems. In 2008, he received the American Physical Society Award for a Faculty Member for Research in an Undergraduate Institution 'for his outstanding contributions to plasma physics made possible by his development of a world-class spheromak laboratory at Swarthmore College, and for his energetic mentoring of undergraduate students'. Professor Brown is a Fellow of the American Physical Society.

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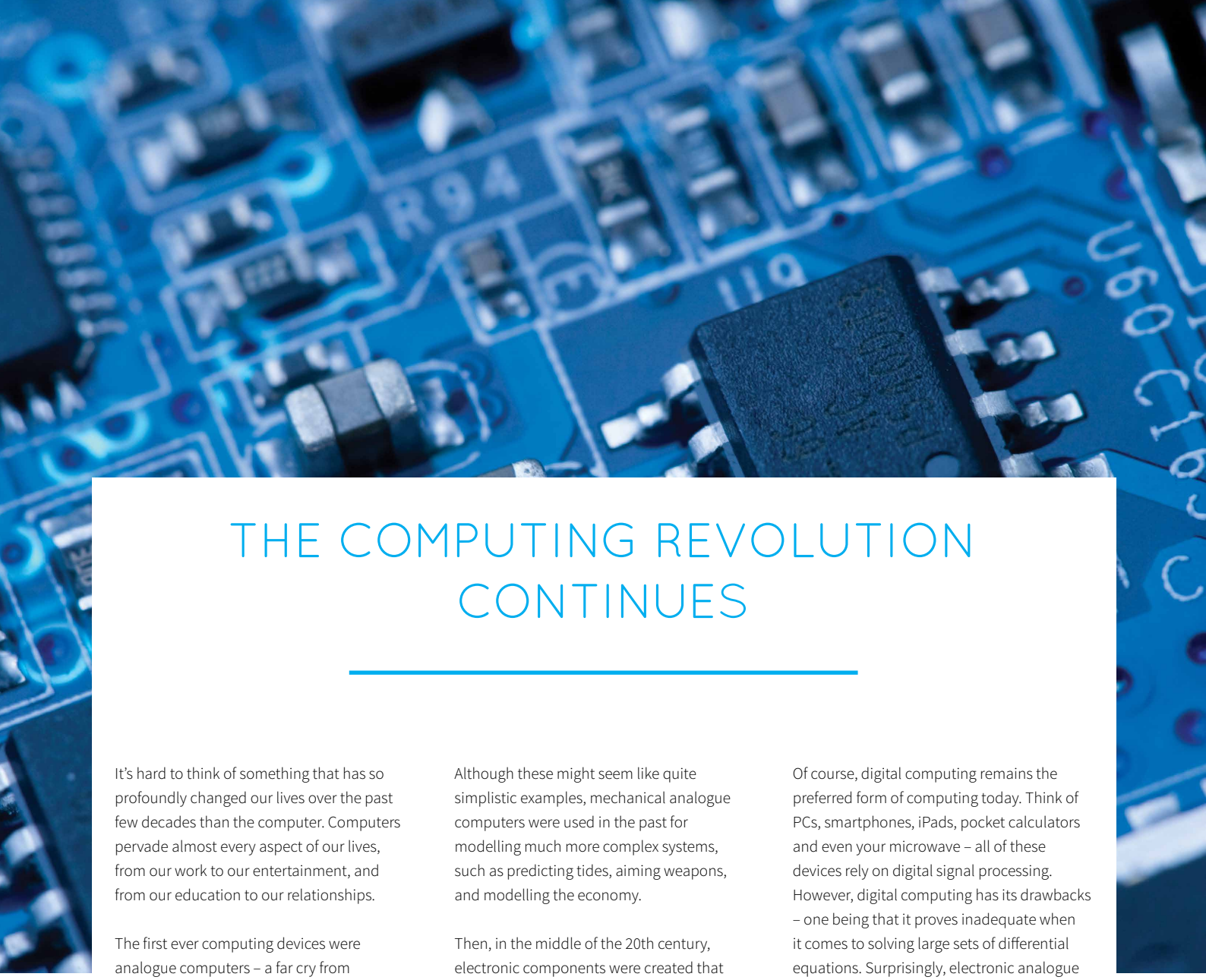
FUNDING

US Department of Energy, ARPA and OFES
US National Science Foundation



THE COMPUTING REVOLUTION CONTINUES

It's hard to think of something that has so profoundly changed our lives over the past few decades than the computer. Computers pervade almost every aspect of our lives, from our work to our entertainment, and from our education to our relationships.

The first ever computing devices were analogue computers – a far cry from today's digital computers – which operated on mathematical variables that were represented by physical quantities such as temperature, pressure or voltage. These early computing devices might shatter many people's notions of what actually defines a computer. Put simply, a computer is a device that – once it has been set up or 'programmed' – can perform calculations independently of the user.

Take a slide rule, for example. This graduated ruler consists of three graduated bars, with a sliding component that allows users to perform many mathematical functions, such as multiplication, division and even logarithms, and is actually considered to be a mechanical analogue computer. Although the slide rule has been rendered obsolete by the digital calculator, many mechanical analogue computing devices are still prevalent today – such as analogue clocks, mercury thermometers and analogue bathroom scales (those with a dial, rather than a digital display!).

Although these might seem like quite simplistic examples, mechanical analogue computers were used in the past for modelling much more complex systems, such as predicting tides, aiming weapons, and modelling the economy.

Then, in the middle of the 20th century, electronic components were created that could be used to accurately perform many different mathematical operations – giving rise to the electronic analogue computer. The 'operational amplifier', for example, could be used to solve differential equation models of dynamic systems. Indeed, during the 50s and 60s, electronic analogue computers were an indispensable modelling tool for technological systems, such as aerospace manufacturing and industrial plant control. However, by the middle of the 70s, electronic analogue computers had been largely replaced with digital systems.

The fundamental difference between analogue and digital computers is the type of data they process. While analogue computers process continuously varying data, digital computers process binary data, which only exists in the form of 1s and 0s. In a digital system, a transistor can only be in one of two states – on and off – while an analogue transistor can be thought of as having an infinite number of states, representing an infinite range of different values.

Of course, digital computing remains the preferred form of computing today. Think of PCs, smartphones, iPads, pocket calculators and even your microwave – all of these devices rely on digital signal processing. However, digital computing has its drawbacks – one being that it proves inadequate when it comes to solving large sets of differential equations. Surprisingly, electronic analogue computers can actually perform these types of tasks with great speed and accuracy.

Therefore, two computer engineers based at The University of Texas in Austin, Dr Michael Bryant and Dr Benito Fernández, propose to build a computer with mixed analogue and digital components – effectively the best parts of both. In the first article of our computing section, we showcase their work to achieve such a hybrid system that can solve very large sets of differential equations. Such a computer could be used to perform accurate simulations across many different fields within science and technology.

Also working to make our current computing technology better than ever before is Dr Balakumar Balachandran and his team at the University of Maryland. In the next article of this section, we showcase his team's research into micromechanical oscillators – components of many electronic systems that ensure data is moved around without becoming corrupted. In particular, they are

exploring how noise can be used to control phenomena within arrays of these tiny mechanical oscillators, in a research project that has implications for drastically improving our current artificial intelligence technologies.

Next, we meet Dr Amnon Besser of Ben-Gurion University of the Negev, who explores p-adic numbers – one of the most difficult concepts in mathematics – in order to solve currently un-solvable equations. Solutions to these equations, as well as techniques developed to solve them, could bring great advances in the fields of computer science, computational physics and algorithms for cryptography.

Our fourth researcher featured in this section of the magazine is Xiaodong Zhang of the Ohio State University. By developing more efficient algorithms, Dr Xiaodong Zhang and his team have successfully revolutionised the design of fundamental computer components. By doing so, they have thus played a key role in improving the performance of personal computers and large computer clusters alike.

Next, we are plunged into that vast ocean of information on every topic imaginable, which much of humanity now relies upon and many of us could not imagine living without – the Internet. To help us find exactly what we need in this immense sea, online searches are becoming increasingly complex. Rather than simple word matching, search engines balance information drawn from multiple sources – not just text from the site being indexed, but also the quality of other sites that link to it, and even the location and search history of the person performing the search. This means that our Internet searches yield immensely more relevant results than just a decade ago. However, although much information is contained within an image or a video, we are still reliant on the text associated with these types of visual media in order to find them in an Internet search.

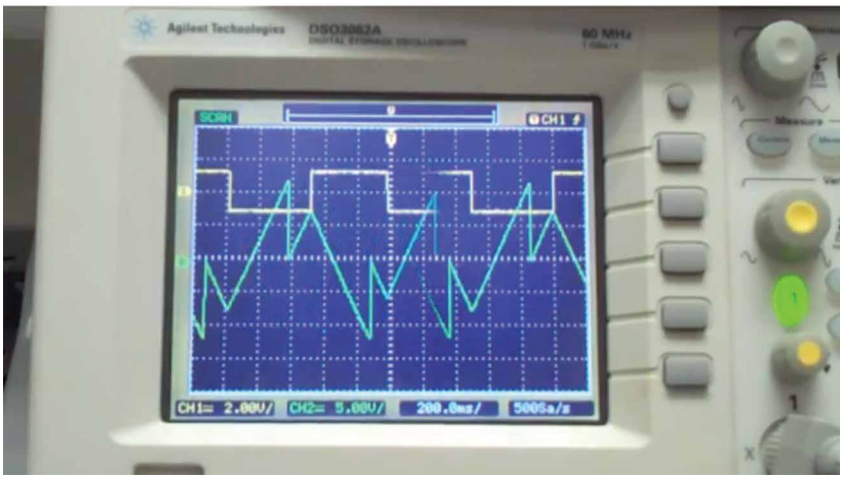
To address this problem, Dr Gerald Friedland and Jaeyoung Choi at the International Computer Science Institute are leading the SMASH program, which aims to improve how we search for visual media online. In the next article of this section, we discuss the team's clever machine-learning techniques, which they employ when training a programme to recognise certain features in videos and images, in order to accurately categorise them and make them much more searchable.

Also making our lives easier through technology is Dr Daniel Jones and his colleagues at Chirp, who have pioneered the development of new software that enables fast, effortless and cheap data transfer using the power of sound waves. In the next article of this section, we detail Chirp's data-over-sound technology, which has been used in numerous applications for wireless communication, spanning sectors from children's games to public transport, and from coffee to industrial powerplants.

Last but certainly not least, we feature a recent breakthrough in controller technology for virtual reality applications. In the field of virtual and augmented reality, one of the biggest challenges that developers face is designing fast and accurate, yet affordable controllers. In this final article of the edition, we meet Dr Christopher Healey and Zeyuan Chen at North Carolina State University, who have announced the creation of CAPTIVE – a controller system they believe will fulfil these criteria. Their technology has the potential to provide enormous benefits to numerous fields, including medicine, architecture, gaming, archaeology and geology, to name just a few.

MIXING ANALOGUE AND DIGITAL COMPUTERS: THE FUTURE IS HYBRID

Differential equations are used to model and describe systems across the whole of science and technology. Current computer designs limit our ability to solve very large systems of differential equations. However, a combination of analogue and digital computing might provide a way to massively increase our ability to do this, opening up a new world of scientific and industrial potential. **Dr Michael D. Bryant and Dr Benito R. Fernández,** along with their colleagues at The University of Texas at Austin, propose to build a computer with mixed analogue and digital components, to achieve a system that can solve very large sets of differential equations.



The Joy of Differential Equations

In the world of mathematics, a differential equation is an equation that relates some important variable(s) to the rate of change of that(those) variable(s). The rate of change is not limited to be with respect to time t, but may include other variables – like spatial variables. A simple example is the velocity of a falling object, which is calculated as acceleration due to gravity, multiplied by the amount of time the object has been falling. In science and engineering, differential equations are often vital in describing the behaviour of components of a system.

Take a car, for example, with its hundreds of moving parts. The movement of these parts can be captured and described using differential equations that link their weight, shape and flexibility to the forces moving them, and to their physical characteristics. So a car engine, or even the whole vehicle, could be characterised by thousands of differential equations, many of which are interlinked with one another.

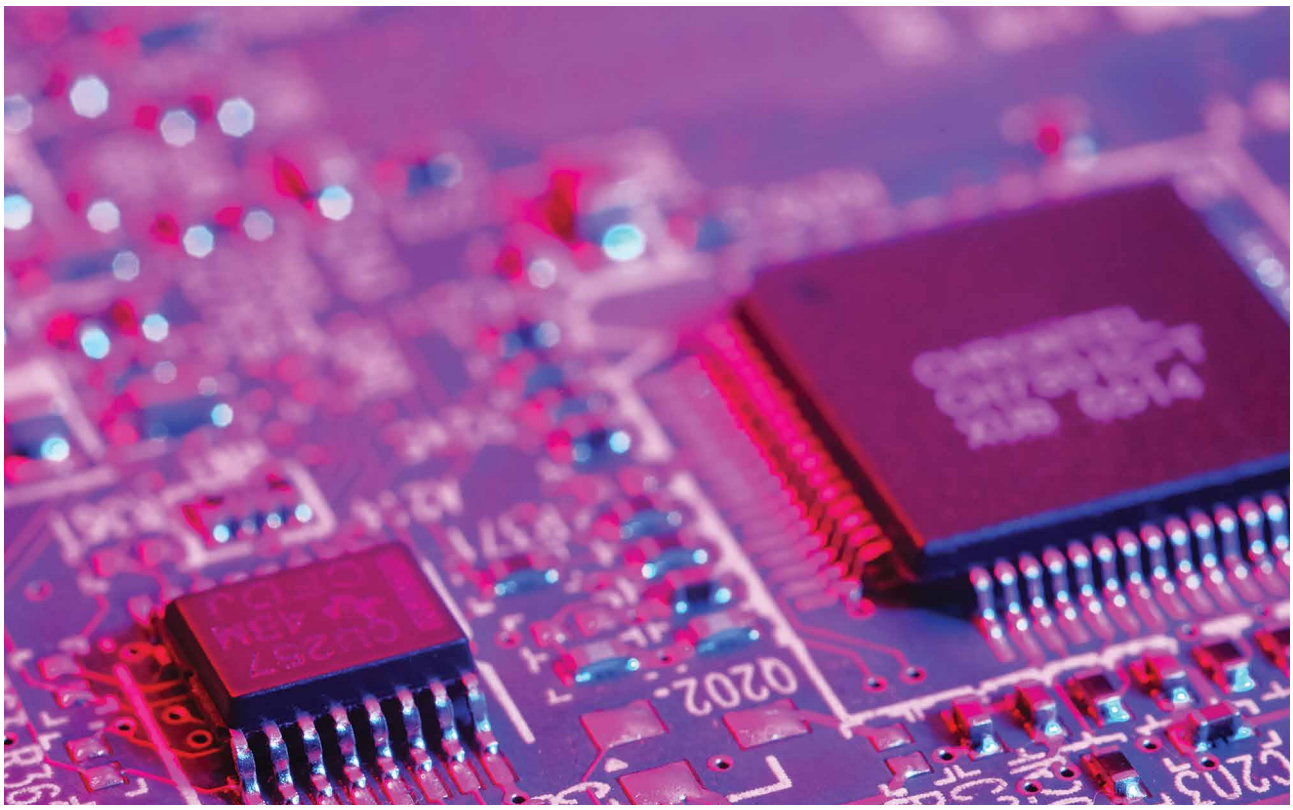
Why is this important? The reason this is a useful way to describe a car is that if you can solve these differential equations, then you can simulate the entire behaviour of the car under any possible set of conditions. You can create a mathematical model of the car, and predict how it will behave, or how it will perform, in any possible situation. If you can do that, then you can identify design problems and solve them without having to spend any money on building and driving expensive prototypes into walls or racing them around test tracks until their engines explode.

This makes testing cheaper and much more reliable, and if this is true of cars then it is also true of oil platforms, fighter aircraft and models of the Earth's climate. In fact, as long as you don't delve too deeply into the tiny details of the universe where quantum effects take hold, just about anything can be treated as a set of differential equations to be solved.

So, what exactly does 'solving' these differential equations mean? A solution to a set of differential equations is another set of equations that precisely defines the variables we are interested in (i.e. speed) in terms of position or some other variables. The unsolved set of equations contains derivatives (the rate of change of variables X with respect to other variables such as Y, Z, U, and possibly time t) that are not useful for any eventual model, but that are unavoidable at the start of the process. At the end of this process, all that remains are the required variables, which can be calculated in relation to one another and exogenous input variables.

The Problem with Digital Computing

Digital computers are amazing. They can carry out billions of calculations every second, on huge numbers of different variables. Since computers can be programmed to find solutions to sets of equations, can they be used to solve differential equations? And if so, is it simply a case of using more computing power to solve larger sets of these equations?



The answer is no – and yes. The computers we all use are totally reliant on binary operations, which can be used to process numbers with a limited number of digits. They cannot be used to completely mimic **real** numbers, and so, some rounding or approximation is unavoidable when they are working with continuous variables, such as speed, distance and time. To achieve sufficiently high levels of accuracy when dealing with continuous variables, digital computers need to be as precise as possible and use lots of significant figures for all the variables, including time, since errors will accumulate as the solution evolves over time. When working with thousands or even millions of parallel differential equations, this means a fantastic number of computations and makes it effectively impossible to find even approximate solutions to these sets of equations in acceptable time frames.

The Problem with Analogue Computing

Analogue computers are effectively 'similar or analogue' models of the system being studied, using some continuous material to mimic the variables being studied, such as electricity or water. Admittedly, once you go down to the quantum level, even electricity and water stop being continuous and turn out to be discrete, but analogue computers operate at a sufficiently large physical scale to allow us to ignore these effects (at the interface between computing and quantum effects, pretty much any statement about the subject is only partially correct, including this one).

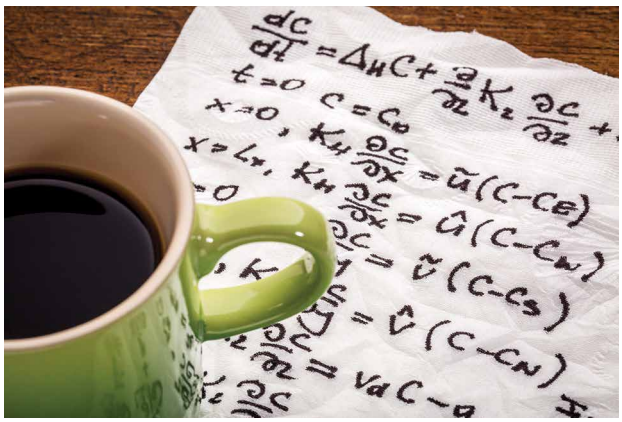
A wonderful example of analogue computing is MONIAC (Monetary National Income Analogue Computer), built in 1949 by Bill Phillips. MONIAC was designed to model the economy of the United Kingdom, using coloured water, pipes and tanks to represent the flow and accumulation of capital throughout the national economy. The concept of MONIAC was parodied by Terry Pratchett in his book Making Money, in which a similar device known as the Glooper not only modelled, but in fact magically influenced the economy it was simulating. The advent of electronic amplifiers led to the creation of electronic analogue computers. By arranging the electronic analogue computer's elements in certain fashion, the circuits would have differential equations identical to those we want to solve.

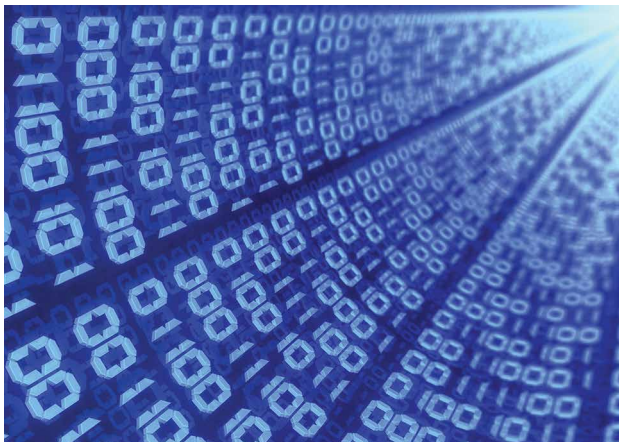
While not actually capable of controlling the systems they are meant to model, analogue computers do have benefits. They can solve systems of differential equations practically instantly, and can do so in ways that allow the processes taking place to be visualised and understood. However, there are a number of problems associated with analogue computing, of which two will be discussed. Repeatability of analogue computers is extremely sensitive to starting conditions. It is impossible to input exactly the same set of voltages into a set of circuits twice, so simulations tend to deviate over time. Also, if the same solution is never arrived at twice, it is impossible to know which one is best. The voltage from the electronic analogue computer, which represents the solution of the differential equation, cannot exceed the supply voltages that feed the circuit. This limits the largest voltage, and thus the largest number the analogue computer can achieve. The solution of differential equations may require large numbers.

Mixed Signal Computing: A Potential Solution?

Because of these problems, analogue computing has never been commonly used, and seems to have become side-lined to a small number of highly specific tasks. Since the explosion of desktop computing in the 1980s, digital computing has been increasingly relied upon as the preferred (although never entirely satisfactory) solution to solving sets of differential equations.

But all this could be changed, due to a new project undertaken by Drs Bryant and Fernández, and their colleagues at The University of Texas at Austin. They propose to build a computer with mixed analogue and digital components, effectively the best parts of both, to achieve a system that can





solve large to very large systems of differential equations. Curiously, Drs Bryant and Fernández have found that the strengths of electronic analogue computers are the weaknesses of digital computers, and vice versa. If they can build this mixed computer, it will cause a significant leap in our ability to simulate large, complex systems in reasonable times.

What the team proposes is an integrated system of mixed-signal integrator cells connected to one another, enabling them to perform complex calculations. Mixed signal electronics combine analogue and digital electronic elements into hybrid circuits. An important part of how these integrator cells operate is that they can represent real numbers completely, rather than simply approximating them to a certain degree of accuracy. The design also allows any continuous function to be approximated, and performs integrations and other calculations without the small 'steps' in value that hamper current digital systems.

So how does this work? The integrated cells combine the binary summation of single small 0 and 1 values as carried out by digital computers, with the continuous flow of signal into and out of containers that represent these small binary values. Let us view the analogue integrator as a cup being filled with 'signal'. If a 'cup' of signal fills up, instead of overflowing as more signal flows in, the full cup becomes a '1' and a digital count of filled cups is increased by 1. Meanwhile the analogue cup resets to 0 or empties and then starts to fill again. Drs Bryant and Fernández named this cup concept an **'analogue bit'.** In this way, the problems of the analogue number limit and the digital number accuracy are solved simultaneously.

The connectivity and functionality of the hybrid integrator cells can be achieved using existing approaches and technologies. However, these novel hybrid components will make it possible for the circuitry to carry out processing simultaneously across the entire interconnected system, in much the same way as an analogue computer operates.

Another innovation of the team's proposed system is that it would be programmable, enabling any system of differential equations to be represented without hard-wiring the system, as with original analogue computers. This means that it can behave in the same way as a digital computer in terms of being programmed, while also having the best qualities of an analogue system and the best qualities of a digital system. As Drs Bryant and Fernández mentioned, the strengths of analogue computers are the weaknesses of digital computers, and vice versa.

Testing the Design

To test this concept and compare it against existing supercomputing systems, Drs Bryant and Fernández created a benchmark problem consisting of one million coupled differential equations. The size of this problem is arguably greater than most systems that would be tackled in current situations and simulation scenarios.

They showed that in comparison to a supercomputer (ASCI Purple) costing hundreds of millions of dollars, their hybrid processing concept was thousands of times cheaper and smaller, while also being significantly faster. This performance comparison was made using modelling rather than a physical system, but was convincing nonetheless.

In addition to the benchmark problem solution, the research team created a printed circuit board (PCB) version of their concept, and used this to verify the design of the proposed system. This PCB was used to check the physical behaviour of the design and to ensure that it operated within expected parameters. In testing, the PCB demonstrated the physical and electronic robustness of the concept and suffered no data or system defects.

The physical size and power requirements of the proposed system are tiny compared to current parallel supercomputers, with the potential for a successful mixed-signal processor to be inserted as a processor on a laptop or handheld device. Such a device would rival current state of the art supercomputing systems in terms of their capability to simulate massive systems of differential equations.

A Hybrid Future

In the future, Dr Bryant and Dr Fernández want to develop their idea further by developing and testing a sequence of increasingly large, complex and sophisticated printed circuit boards containing integrator cells, and integrated circuits with hundreds or thousands of integrating cells. They also want to develop a system to control and program this through a computer. Future versions would have an in-built operating system allowing the circuitry to be programmed directly, with the circuit board integrated as an insert into a laptop or handheld device.

If successfully developed, such a device could be used to rapidly improve a large number of activities reliant on solving huge sets of differential equations. These include weather forecasts, maintenance diagnostics, virtual reality simulation and system design. Also, such a system could be used for neural network and AI-based applications, as neural networks are effectively large interconnected sets of nonlinear differential equations.

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After obtaining a BS in Bioengineering from the University of Illinois at Chicago in 1972, Dr Michael D. Bryant achieved a Masters in Mechanical Engineering at Northwestern University in 1980 and a PhD in Engineering Science and Applied Mathematics from the same university in 1981. He worked at North Carolina State University as an Assistant Professor from 1981 to 1985, and then as Associate Professor from 1985 to 1988. Since 1988 he has been a Professor at the University of Texas at Austin, and is currently Accenture Endowed Professor of Manufacturing Systems Engineering. His research focus includes mechatronics and tribology. Dr Bryant has over 100 published peer-reviewed publications, book chapters and conference papers, and several patents derived from his research. He is a Fellow of the American Society of Mechanical Engineers and is a member of the Institute of Electrical and Electronics Engineers and several other Societies.

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Dr Benito R. Fernández began his career in Venezuela, where he studied Chemical Engineering in 1979 and Materials Engineering in 1981. In 1981, he moved to the US to carry out graduate research at MIT, where he received his MS in 1985 and PhD in 1988, both in Mechanical Engineering. Dr Fernández specialises in Applied Intelligence – in particular the use of different technologies to create intelligent devices and systems. He is also an expert in Nonlinear Robust Control and Mechatronics. His research focusses include manufacturing automation, industrial equipment diagnostics and prognosis, evolutionary robotics, hybrid Processors, eXtreme (resilient) devices, cyber-physical systems, smart energy systems and mechatronic design. Dr Fernández is the founder and Director of the NERDLab (Neuro-Engineering Research & Development Laboratory) and the LIME (Laboratory for Intelligent Manufacturing Engineering).

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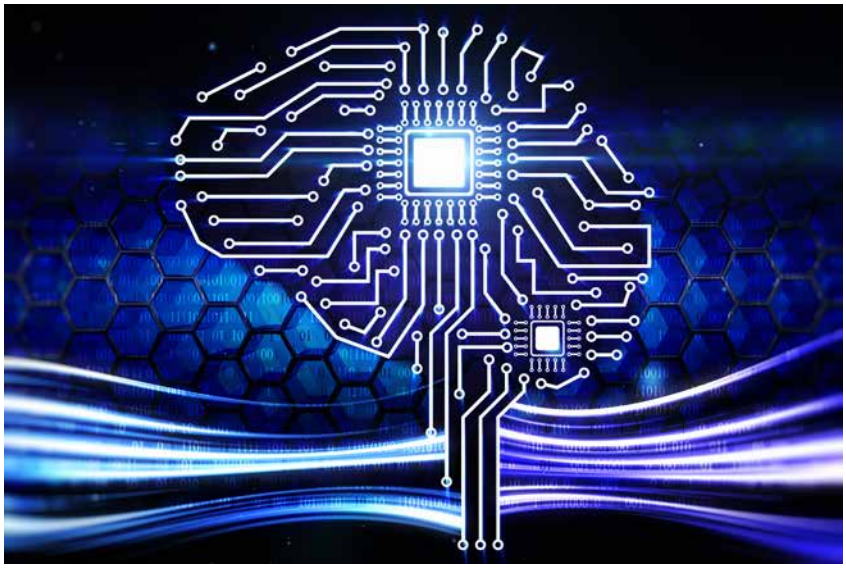
FUNDING

National Science Foundation

TEXAS
The University of Texas at Austin

USING NOISE TO CONTROL MICROMECHANICAL & MACROMECHANICAL SYSTEMS

Micromechanical oscillators are components of many electronic systems that keep track of signal processing and ensure data is moved around without becoming jumbled up. **Professor Balachandran** and his team at the University of Maryland are exploring how noise can be used to control certain phenomena within arrays of these tiny mechanical oscillators, to change their behaviour and make them operate better than before. Their studies also have important ramifications for macro-scale mechanical systems.

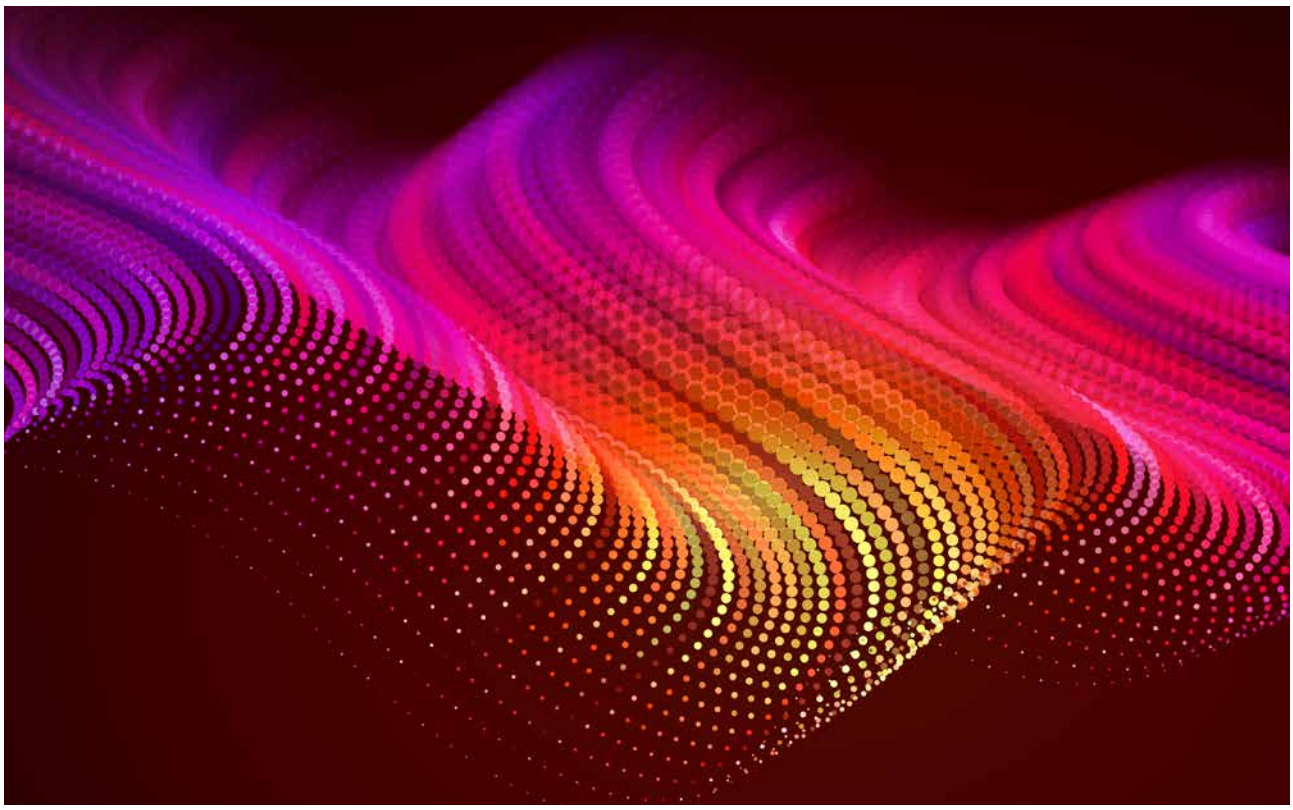


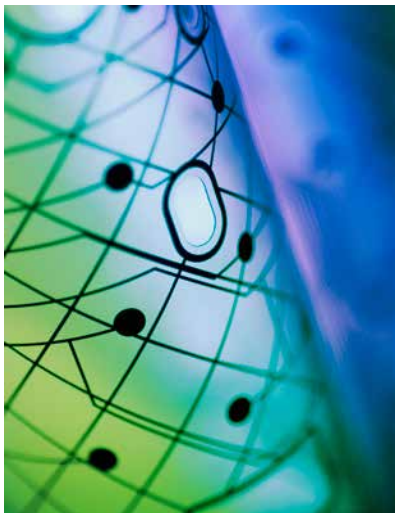
At very small scales – those smaller than a millionth of a metre – strange effects and phenomena can be observed in dynamic systems. These effects are usually not observed at larger scales, or are so tiny that they become swamped by everything else taking place. Some of these effects appear random in their cause, but can be attributed to fabrication flaws in the very small components of a system. Sometimes, vibrations caused by thermal sources can cause these components to start exhibiting unexpected activity (heat, at the smallest scales, is after all just vibrations of atoms and molecules).

However, for the design of systems that have very small components – for example, integrated circuits – a better understanding of these strange phenomena is needed. This is true not only so that people can know how the system will behave, but also because these phenomena could potentially be used to control micromechanical systems and make them perform in entirely new and better ways.

One type of system that has components small enough for these effects to take place is a micromechanical oscillator array. Micromechanical oscillators are tiny devices that generate electrical or optical signals with very accurate frequencies. Effectively, they act as miniature clocks within more complex systems, and these systems can be used to carry out a number of different functions. Quartz crystals used to be the standard for generating regular frequency signals within a system, but they are sensitive to impacts and can easily be disabled or made inaccurate. In the last decade, more robust oscillators have been fabricated from different materials and have more sophisticated designs. Much of the early work in this area was funded by DARPA, the US Defence Advanced Research Projects Agency.

One of the most important of these oscillators is timekeeping, in order to keep track of signal processing within the circuitry and ensure that data is moved around without becoming jumbled up. In effect, these oscillators provide a heartbeat for the rest of the electronic system. Where multiple timing signals are required, a number of oscillators are often placed together in orderly arrays. At the University of Maryland, Professor Balachandran and his research team have been working for several years to understand the effects of noise and vibration on the behaviour of oscillator arrays across different length scales. Impressively, the team has figured out new ways to control these effects.





The Bizarre World of Intrinsic Localised Modes

Intrinsic Localised Modes (ILMs) are a phenomenon that takes place in these arrays of oscillators, where energy accumulates in a spatial region or wave within the system. Usually, this localisation occurs at a single location and holds position, which is different from what would be expected in a classical wave system – normally the energy is dissipated away from local sources and the wave travels through the system. For this reason, ILMs are also sometimes called breathers as they 'breathe' in and out, usually holding steady at one location. However, under certain conditions, they can also move through an oscillator array without dispersing the wave energy – a phenomenon with many potential applications if it can be controlled.

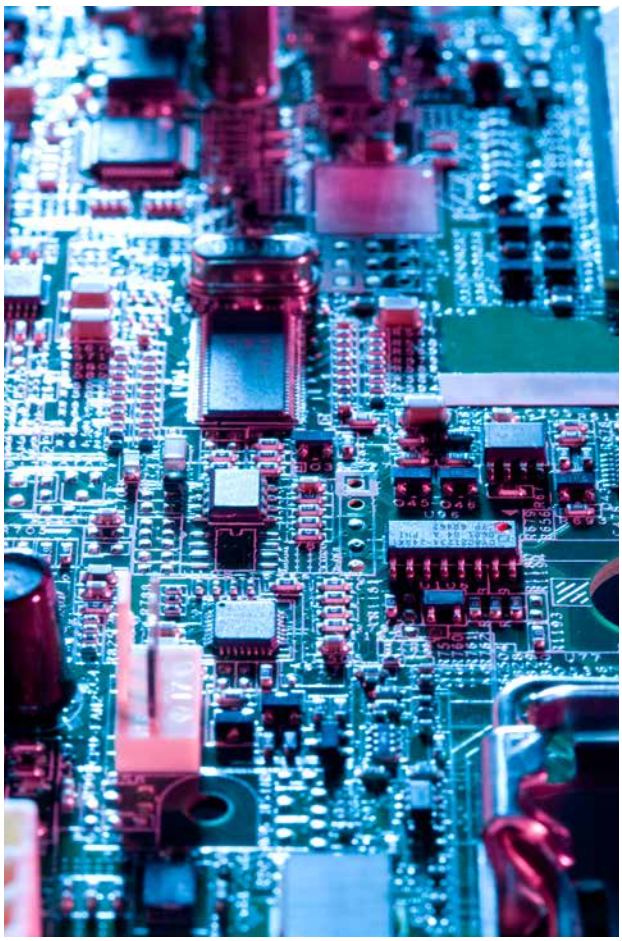
The reason that ILMs exist in oscillator arrays and other similar systems is difficult to pin down and still a topic of many research investigations. Originally, they were thought to result from random noise within the oscillator system, but this was shown to be impossible. However, Professor Balachandran and his colleagues have shown that with sufficiently high intensity noise of the correct type and frequency content, ILMs can be variously generated, enhanced or suppressed throughout an oscillator array. Developing this ability to control ILMs is important, as it might give rise to new and useful behaviour within the array.

Noisy Oscillations – Better than the Normal Kind?

This control is achieved by adding noise to the baseline signal controlling the array, with the effect of this depending on the strength of the noise in relation to the baseline signal. What Professor Balachandran and his team have found is that it is possible to make ILMs occur at specific, controlled locations within in the oscillator arrays, and also to make them last longer than they normally would.

In addition to this, the team has explored the effects of signal noise on the creation and destruction of a specific type of ILM, within arrays of oscillating cantilevers that are coupled to one another. These cantilevers, which are beam oscillators held at only one end by a coupling rod, were vibrated from side to side, while the team measured their responses by using strain gauges. When they added noise to a harmonic input with a certain vibration frequency, an intrinsic localised mode (ILM) was generated. The team found that in the absence of noise, no ILM was present in the system. They also found that when noise was added to a system where an ILM existed, it destroyed the ILM.

The frequency and strength of the signal driving an array of coupled oscillators appear to be two important factors in the creation of ILMs. The strength of the noise signal is also vital in terms of its influence on the ILMs. However, the relationships that exist between all these factors are not yet properly understood. In order to investigate further, Professor Balachandran and his colleagues have developed a macro-scale mechanical system that mimics arrays of tiny oscillators by using cantilever oscillators, enabling them to control the frequency content and level of noise added to the system.



Useful Noise

There are multiple applications for this work ranging across a number of fields, beyond engineering. One of these is artificial intelligence, where adding noise to the input signals of artificial neurons can enhance and improve the signal-processing performance of the system. It seems strange that adding random fluctuations to the input signal would result in better and more stable pattern recognition within an artificial neural network, but researchers have validated this mathematically.

Without noise in an artificial neuron's signal, it tends to become stuck in one of the two possible states (active or inactive). With too much noise, the neuron fires randomly and provides a meaningless output. But with the right amount of noise added to its input signal, the artificial neuron becomes much more capable of swinging between these two states when it needs to, with a greatly reduced background signal. This makes it more responsive to changes in this signal and improves pattern recognition.

The mathematics explaining this and other effects within an array of oscillators is quite complicated, but at its core, it is based on the Fokker-Planck equation. This equation describes how the velocity of a particle or an object will change over time, when it is subjected to drag (dissipation) and random forces. The Fokker-Planck equation is a partial differential equation, meaning that it combines values of parameters with the rates of change of those parameters. This makes the equation exceedingly difficult or impossible to solve for nonlinear systems, except under special circumstances.

When there is no solution to a specific mathematical equation, researchers normally rely on simulation methods to approximate variations of the value over small distances. This is a bit like splitting a simulated volume up into lots of small boxes, and calculating the change to the values in each box over small time steps. With the Fokker-Planck equation, this approach allows the particle movement to be changed from a continuous smooth curve to a series of tiny steps. If the steps are small enough, then this gives the same appearance as a smooth slope when viewed from a distance.

For simulations of coupled oscillating systems, the Fokker-Planck equation demonstrates what is seen in reality – that the oscillating system tends to become stuck in specific patterns. Adding noise to the equation, as in real life, shows that the system is much more capable of switching between states and therefore responding in a much more sensitive manner to external stimuli. This finding has relevance for sensors and signal processing, and has even helped to explain a number of observed biological phenomena, such as the foraging behaviour of animals.

The challenge is to figure out the best possible way to apply noise within a coupled oscillatory system, in order to maximise the benefits of this effect. Professor Balachandran and his team have explored this with their mechanical cantilever oscillator array device, which allows them to alter the frequency of the harmonic signal and the relative strength of the noise added. The cantilever, if left to itself, tends to switch back and forth regularly and repeatedly between the two states without any variation. When the team adds noise, the cantilever tends to stabilise around an equilibrium or fixed point, oscillating much less than before.

Further Work

What Professor Balachandran and his team have found is that this noise can be used to steer the performance of an oscillating system towards a desired dynamic state. The earliest observations of this were found in microscopic systems, but the results of Professor Balachandran's research have enabled this phenomenon to be translated into macroscopic systems. This is an important point, as it implies that we may be able to gain better control over complex oscillating systems and enhance their performance. However, there is still much work to be done in this area.

Professor Balachandran and his team have developed an analytical-numerical framework that enables them to study the effect of noise on the dynamics of coupled oscillating systems. Along with the mechanical system they have constructed, this will allow the team to explore various arrangements of the system, vibration, and noise. They will also be investigating ways to scale up some of the phenomena observed in arrays of microscopic oscillators, to see if they can be induced in macroscopic systems. One future study of interest to them is a rotor system whose dynamics they expect to influence by injecting noise into the drive torque.

In addition, the team plans to develop an experimental prototype containing other types of oscillators, and to experiment with more sophisticated models of coupled oscillating arrays. This will allow them to gain a better understanding of how real-life coupled oscillatory systems such as artificial intelligence designs could be improved, and even controlled.

Meet the researcher

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Professor Balakumar Balachandran received his PhD in Engineering Mechanics from Virginia Tech, USA. Since 1993, he has worked at the University of Maryland, where he is currently a Minta Martin Professor of Engineering and the Chair of the Department of Mechanical Engineering. He is a Fellow of ASME (American Society of Mechanical Engineers) and AIAA (American Institute of Aeronautics and Astronautics) and is also a member of several other societies. His research interests include nonlinear phenomena, dynamics and vibrations. Much of his work has focused and is focused on nonlinear phenomena, dynamics of nonlinear systems, and control mechanisms for nonlinear systems. His team's recent work has included efforts to use nonlinear phenomena for the benefit of system control. Professor Balachandran has published over 90 journal articles and a number of textbooks and book chapters related to nonlinear dynamics and vibrations. He serves as the Technical Editor for the *ASME Journal of Computational and Nonlinear Dynamics*, a Contributing Editor of the *International Journal of Non-Linear Mechanics*, and is on the editorial boards of several journals including *Acta Mechanica Sinica*, the *Journal of Vibration and Control*, and the *International Journal of Dynamics and Control*.

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FUNDING

US National Science Foundation
(Grant Numbers: CMMI-0800471, CMMI-0826173, CMMI 1436141, CMMI1436141)

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UNIVERSITY OF MARYLAND

MAPPING *P*-ADIC SPACES WITH HEIGHT PAIRINGS

Professor Amnon Besser of Ben-Gurion University of the Negev and his colleagues are exploring *p*-adic numbers – one of the most difficult areas of number theory – in order to solve long-standing open problems bridging several fields of mathematics.

Solving Unsolvable Equations with a New Number System

If you are somewhat familiar with advanced mathematics, specifically number theory, it is likely you have heard of *p*-adic numbers. Often spoken of with reverence, and described as one of the most difficult areas in pure mathematics, *p*-adics are regarded as inaccessible to the public. However, they have many real-world applications, such as encryption algorithms, and have the potential to solve several problems in fundamental physics through theories such as *p*-adic quantum mechanics. The modular way in which *p*-adics retain information about the equivalence between different numbers is fundamental to the demonstration of Fermat's Last Theorem, as discovered by Andrew Wiles no less than 350 years since Fermat first stated it. In fact, the consequences of the *p*-adic number system stretch far beyond that. Although they started as a natural quirk derived from the need to solve Diophantine equations (polynomial equations in which only integer solutions are allowed), it is believed that they have deep implications touching upon the Birch and Swinnerton-Dyer conjecture and the Riemann Hypothesis – two open Millennium Prize Problems.

For Professor Amnon Besser of Ben-Gurion University of the Negev, *p*-adics have been a source of hope for finding a specific answer to a computational problem. Part of his problem involved an integration method developed by Robert Coleman, a method which is the *p*-adic equivalent of integration along a curve between two points. After his PhD, Professor Besser often used Coleman integration while delving into *p*-adic number theory. Later on, he heard that algorithms that compute a function called *p*-adic height could have important applications in cryptography. At that time, such an algorithm had already been produced, but Professor Besser felt he could create a better, more general one. Later on, he joined forces with Jennifer Balakrishnan, who was working on finding certain solutions specific to computing Coleman integrals. Their work produced a new method for computing a function called a *p*-adic height pairing, and facilitated the generalisation of Professor Besser's previous results.

Now, a large part of Professor Besser's research focuses on using numerical methods to find rational solutions of algebraic equations. Developing numerical methods can address situations where no exact solutions are known for a class of equations, by reducing the problem to number crunching. In general, these types of numerical solutions can help scientists and engineers when dealing with an ill-behaved function that models an aspect of applied research.

In order to have a better understanding of these problems, let's go back to the basics of *p*-adic number theory.

What Are *P*-adics?

P-adics were created from a desire to apply the techniques of power series methods to number theory, as a way to express certain numbers or mathematical problems in a tractable way. After all, number theory, or the queen of mathematics as Gauss called it, is famous for posing some of the most difficult conjectures in the entire field of mathematics. Thus, the idea to create tools that would transform intractable problems into approachable ones is a very natural strategy.

Just like complex and real numbers, *p*-adic numbers extend the rational number system Q and its associated arithmetic operations. If rational numbers can be expressed as a ratio between two integers p/q, real numbers are expressed as an endless decimal expansion. One such number is π and another is √2, and even 1 can be written as 1.000… or 0.999… for example, which is a sum of an infinite number of powers of 1/10. Unlike real numbers, *p*-adics are expressed as sums of powers of a prime number, usually denoted by p. Since the letter p is simply a placeholder for the base, replacing it with some number will yield base-dependent names like 2-adics or 17-adics and so on.

In a way, *p*-adic numbers are the opposite of real numbers. The difference derives from the ordering or closeness within the number system. If two real numbers that differ in the 10^{th} decimal digit are closer than two other numbers differing in the 2^{nd} decimal digits, for *p*-adics the concept of closeness is a much more interesting one. Albeit counterintuitive, this is thoroughly consistent within the *p*-adic number system. Thus, *p*-adics are close when their difference can be divided by a high power of p. The higher this power is, the closer the two numbers are said to be. In our example where p is a fixed prime and e a variable power, the difference between *p*-adics is divisible by pe and the numbers are close when e is very large. In other words, two decimal

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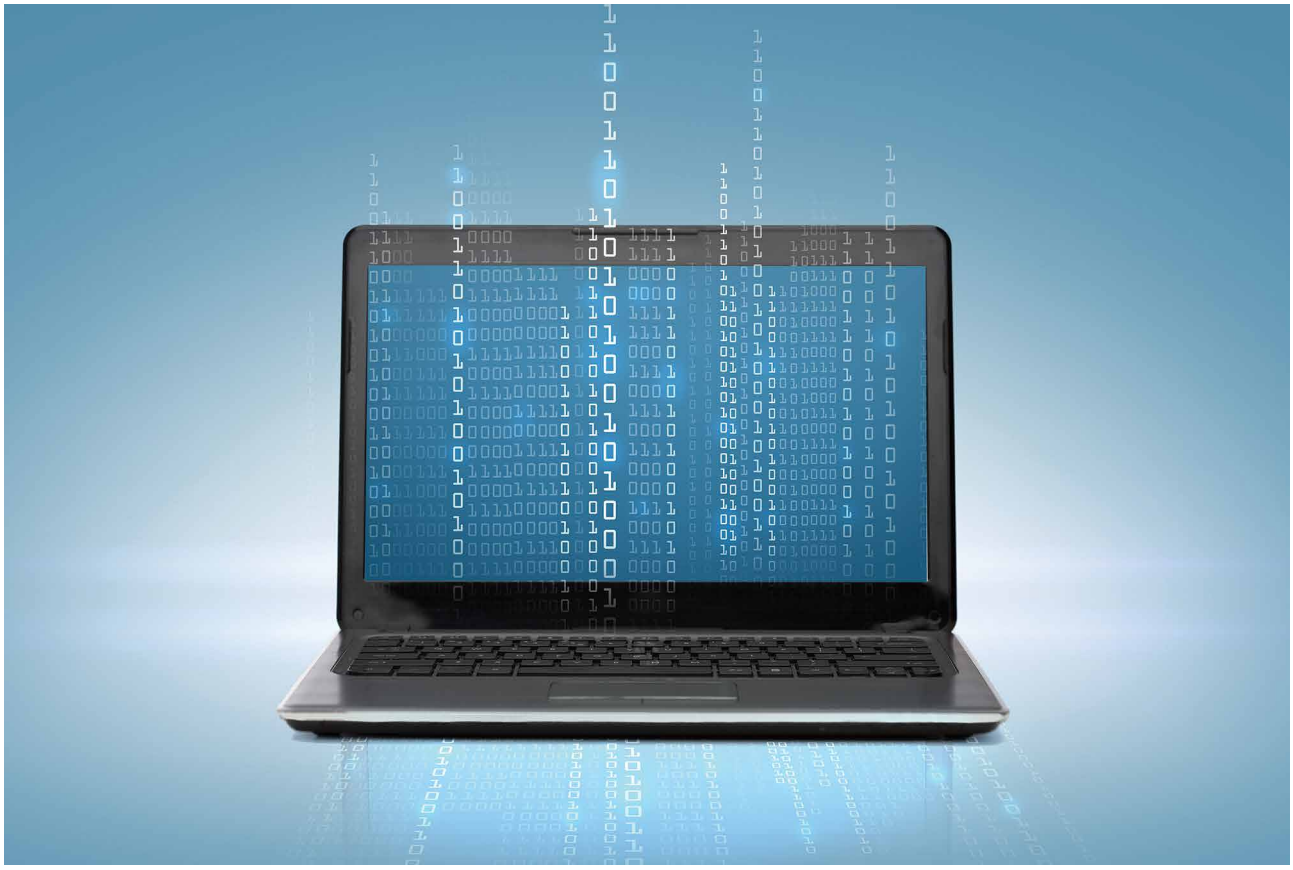


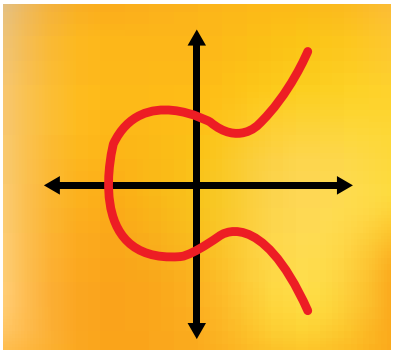
representations of a real number are close when the difference between them is a large negative power of 10, whereas two *p*-adic expansions are close when their difference is a large positive power of p. For *p*-adics, the concept of closeness opens the possibility to encode information about congruence of absolute value, which could be called their measure, in a new and interesting way.

In addition, *p*-adics can be considered opposites of real numbers in terms of their representations. Due to change of base, *p*-adic numbers are written from right to left, each digit added to the left increasing the precision of the number representation. Recall that expansions of real numbers are written the other way around, from left to right, with a finite number of digits before the decimal point and an infinite number of digits after it. *P*-adics, on the other hand, can have an infinite number of digits to the left. Moreover, the *p*-adic number system is based on the modular number system, like a clock that resets to zero when reaching 12-midnight, which means that the arithmetical operations behave differently from those of usual arithmetic. One reason why *p*-adics are a particularly neat number system is that the base must be a prime number, otherwise the set of all numbers obtained from arithmetic operations is not closed under these operations. In other words, you can divide *p*-adics with a non-prime base and get a number that was not part of the initial set.

Mapping the Path to Unique Solutions

Although *p*-adics in particular and number theory in general seem to be purely abstract mathematics, they are both born of the very simple goal of solving equations. As Professor Besser explains, ‘I look for new methods for solving equations. I put the usual well-known numbers inside some bigger space from which one can cut out the pieces containing the solutions.’

These equations are important for all types of applied problems in physics, engineering, finance, and other fields. In their simplest



Elliptic curve

form, the Diophantine equations that led to the development of *p*-adics can be written as $ax + by = c$, where x and y are variables and a, b and c are constants. In addition, *p*-adics methods can be used to study superelliptic equations, where $y^m = f(x)$, and hyperelliptic equations of the form $y^2 = f(x)$. The representations of these equations are often called curves in the formal language of mathematics due to their shape. Sometimes, these curves self-intersect to form a closed boundary.

The only solutions in integers to

$$y^2 = x^3(x-1)^2 + 1.$$

are $(2,\pm 3)$; $(1,\pm 1)$, $(0,\pm 1)$.

One of the peculiarities that follow from the rules of *p*-adics is that they cause unusual behaviour. In a geometric interpretation, *p*-adic numbers form a space much like the Euclidean flat space in which we live. However, their space has a completely foreign definition of the distance between two points, called a metric. In this space, the triangle inequality is stronger than in flat space. As Professor Besser points out, one consequence of this is that 'any two circles are either disjoint or one contains the other.' Because of this property, functions such as integrals, when defined over complex numbers, can be extended beyond their normal domain by creating analytical paths and moving from one point to the next. This technique, called analytic continuation, allows mathematicians to find rigorous answers to otherwise intractable problems, such as extending functions over singularities or summing certain series. However, these techniques conceal a trap in complex spaces. When following the analytic continuation of a function, the calculation may descend into a loop and retrieve multiple values for the same calculation. However, the strange behaviour of *p*-adic spaces does not support analytic continuation at all, resulting instead in a huge multivaluedness, too large for practical purposes.

Professor Besser found a way to overcome the problem of multi-valued results for the same function by continuing Coleman's work on integration. Recall that Coleman worked on defining the equivalent of integration under a curve for *p*-adics. Professor Besser interpreted Coleman's ideas in a way that led to a formal definition of paths. By making certain assumptions about the way in which the functions transform along the paths, 'these paths live on a discrete structure obtained by shrinking all the small circles in the *p*-adic world to points,' as Professor Besser explains. In this way, instead of working with a discrete space where functions would jump between circles, he went on to recover the continuum in the limit of the circles tending to zero. Moreover, the same operator that remembers how functions transform along the paths also maintains them as fixed and allows for unique answers to be found, thus eliminating the problem of multi-valued results. Although they are more difficult to define, Coleman integrals are better in some cases than complex integrals because they are single valued.

Meanwhile, Professor Besser's colleagues, including Minhyong Kim from Oxford, used a non-abelian generalisation of a method devised by Claude Chabauty in 1941 to find rational-valued points on curves with special properties. The Chabauty method allowed them to progress in theoretical directions, by showing that some Coleman integrals become equal to zero on rational solutions of certain equations. This important finding proved that these integrals have a finite number of solutions, because a Coleman integral can become 0 only a finite number of times.

During this time, Professor Besser focused on the practical question of actually finding the rational and integral solutions to equations using the Chabauty method. His approach involved using *p*-adic height pairings. The approach is based on the idea that rational solutions to equations can be added together in some sense. The advantage of the *p*-adic height pairing is that it transforms in a very simple way when solutions are added, and this leads to equations on the values of the height pairing at integral points. Based on Professor Besser's previous work, these equations can be expressed as a Coleman integral becoming zero. Although this seems like a simple enough exercise, there are in fact many categories of unsolvable equations. Solutions to these equations, as well as techniques used for their solution, could bring great advances in computer science and computational physics. 'One of the key points in the computation of Coleman integrals is the Kedlaya algorithm, which finds the number of solutions of certain equations modulo a prime p, a problem whose primary motivation is in the field of elliptic curve cryptography,' Professor Besser tells us. Recall that elliptic curves are representations of algebraic elliptic equations. Plotting the points of these equations results in curves which often self-intersect, forming a closed boundary. Elliptic curve cryptography uses such equations to generate much shorter secure public keys than those generated using other methods.

Professor Besser hopes to extend *p*-adic height pairings to more general cases and use them to solve badly behaved equations. The latter is an important step in understanding the relevant mathematics in a fundamental way, and in solving some of the most interesting open problems of the field.

Meet the researcher

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Professor Amnon Besser currently holds a research position at the reputed Ben-Gurion University of the Negev in Israel, where he has been teaching since 1999. His research interests span number theory, *p*-adic integration and cohomology, Shimura varieties, automorphic forms, algebraic cycles and K-theory. Besser received his PhD in 1993 with a thesis in number theory on Universal families over Shimura curves. Throughout his career, he has held research positions in several famous institutions, such as Oxford University, Princeton, the Max Planck Institute for Mathematics, UCLA, and Arizona State University. He has authored over 30 papers that have been published in journals and presented at international conferences. From the standpoint of productivity and overall impact, his work has a calculated h-index of 8. Recently, he has been researching *p*-adic height pairings and integral points on hyperelliptic curves.

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FUNDING

Israel Science Foundation

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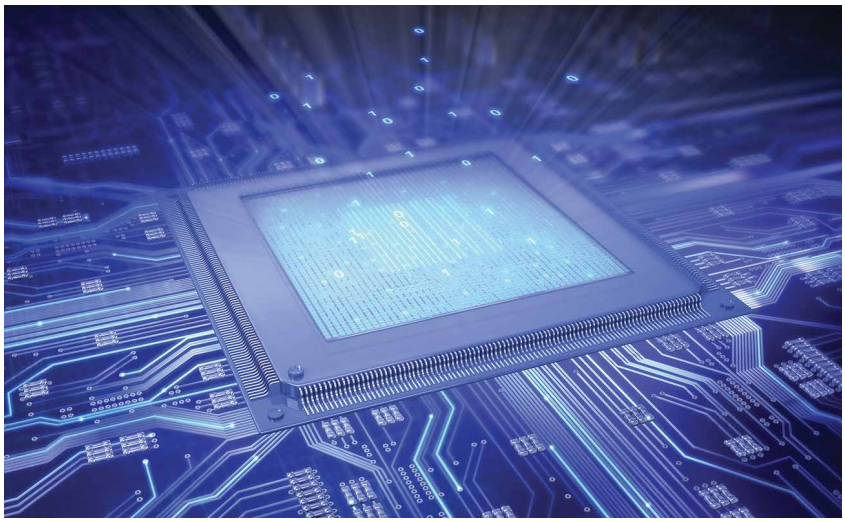
Ben-Gurion University of the Negev

ALGORITHMIC ACCELERATION OF COMPUTING PERFORMANCE

The endless quest for making faster, more powerful computers is not just about investing in advanced hardware. By developing more efficient algorithms, **Professor Xiaodong Zhang's** work has successfully revolutionised the design of fundamental computer components. By building upon basic computer science research on memory management processes, Professor Zhang has played a key role in improving overall computer system performance, not just for individual personal computers but also large computer clusters for data management systems.



Although loading a program to run on a computer might only require a few clicks from the user, there is a complex cascade of processes that are occurring while you wait. Your input from the mouse or a touch screen sends an electrical signal that is received by the computer's central processing unit (CPU). The CPU is like the computers 'brain', that allows it to respond to inputs, like mouse clicks, and executes the lines of code that make up a computer program. However, when you are trying to run a computer program and open its related data files, the code and data need to be stored somewhere, which is typically on the hard drive of the computer. This means that the CPU needs to access the data on the hard drive and find the correct program before it can even start running the program itself.

To run the program, a copy of the program and necessary data are first loaded into the main memory or DRAM (Dynamic Random Access Memory). Unlike a hard drive, where data is stored permanently, DRAM is a type of temporary storage. If you reboot your computer, then any data that is stored in the DRAM will be lost. The reason DRAM is used to store a copy of the program is because it is significantly faster to read from and write to DRAM compared with hard drive storage, ultimately meaning your program will run much more smoothly.

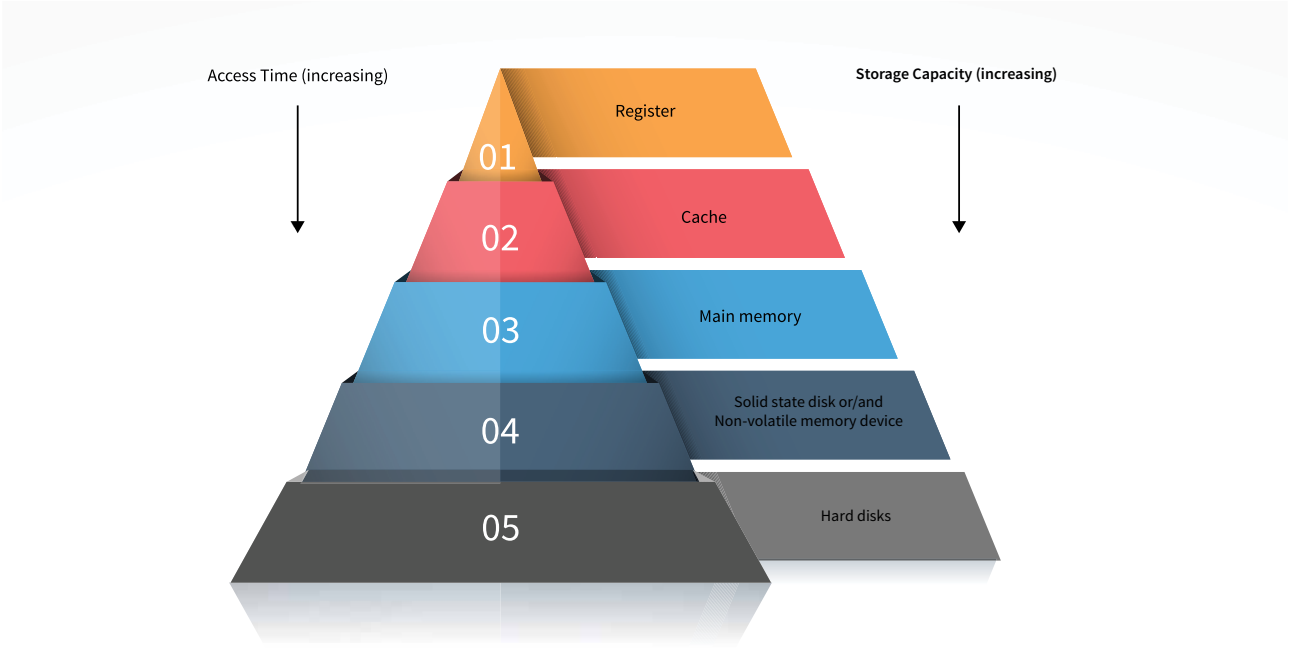
Every step in running a program requires communication between, and access to, several different kinds of memory in a hierarchy from fast to slow. Your operating system, be it Windows, Linux, OS X or Android, is continuously running on the CPU and helps to not only provide an interface for you to interact with but to translate various commands to and from the CPU and various parts of memory. It also tries to manage the overall memory usage of the computer.

Loading, Please Wait…

The continual 'back and forth' of commands between the CPU, hard disk and DRAM means that there are various stages at which 'bottlenecks' can occur, which limit the overall performance of a computer. For example, some types of computer programs, such as graphically-rich video games, are very 'DRAM intensive', so even with a significantly faster CPU, if your DRAM is insufficient, they may run sluggishly. While these bottlenecks may occur in individual components, a more significant and common source of bottlenecks is delays in the communication between the various kinds of memory.

One approach to solving this is to increase the memory capacity and upgrade CPU speed in the hardware. However, this is costly in terms of resources and it is becoming increasingly difficult to keep producing smaller and smaller transistors for CPUs, due to complicating factors such as the amount of heat produced. The most critical issue is to maximise every bit of potential of hardware by the power of algorithms. Where Professor Zhang and his research team excel is in finding different algorithms to optimise many of these 'memory management' processes. This ultimately means that you can see faster system performance using the same specification components by finding ways to make their operation or the communication between components more efficient.

‘Data accessing speed to the main memory is a critical factor for computer system performance. By translating basic research into advanced technologies, we have been able to have a huge impact of the development of the both the hardware and software components of computer systems.’



Reducing Conflict to Accelerate Memory Access

Every communication process, or attempt to read or write data from memory, has a certain probability of causing an error. There can also be inefficiencies caused by the order in which data is written to and read from memory.

For modern DRAM systems, one of the biggest inefficiencies is caused by row-buffer conflicts. In order to speed up memory access, the memory is divided into different ‘banks’, each of which contains multiple ‘pages’, a standard data unit, e.g. 8192 Bytes. Each bank has an associated row-buffer, which keeps data in memory so it can be re-accessed to speed up processing times.

However, sometimes an event called a ‘row buffer conflict’ occurs, which leads to a substantial delay in memory access. This is when there is an attempt to access a page while another page is already open in the row-buffer. To address this, Professor Zhang, with two of his former PhD students (Zhao Zhang and Zhichun Zhu, who are both now professors at the University of Illinois at Chicago) developed an algorithm known as ‘permutation-based page interleaving’ that significantly reduces the likelihood of these row-buffer conflict events.

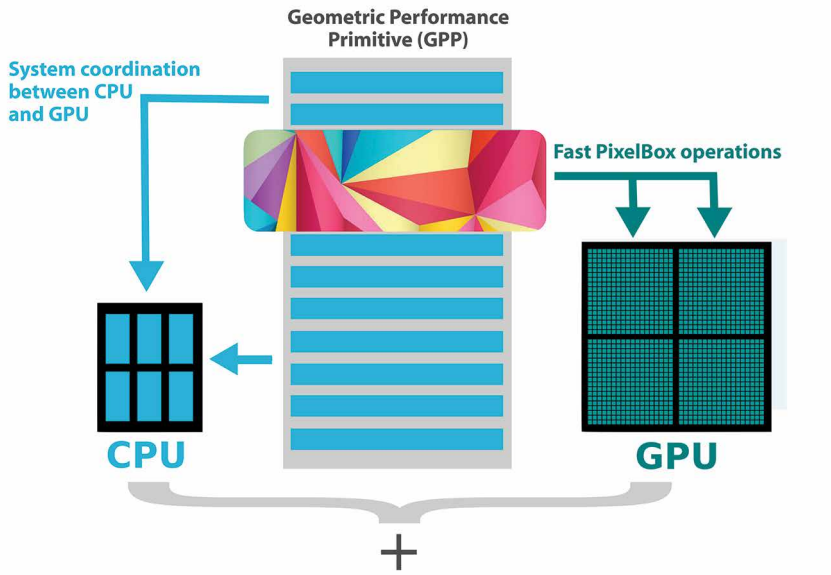
Use of Professor Zhang’s new algorithm has reduced memory access time significantly. This method has proved so useful that it has been adopted in almost all the general-purpose microprocessor products, originally by Sun Microsystems, and later by AMD, Intel and NVIDIA. It is now considered part of the conventional design of the memory controllers that make up the microprocessors to form the CPU.

To Keep or to Evict?

In any computer system, there are several layers of data buffers known as ‘caches’ in a hierarchy, used to store information the CPU is likely to need, reducing the time taken to access data from the next level of the memory hierarchy. For example, accessing data in CPU caches is much faster than in the main memory, and this trend continues until the last level of the hard disk is reached.

The question is, how do you identify what data is likely to be used often and what should be cached in order to speed up processing? This is normally done algorithmically, where the data is removed from the cache based on which data was ‘least recently used’ (LRU). However, now Professor Zhang, along with another former PhD student, Song Jiang (now a professor at the University of Texas, Arlington) have co-developed the Low Inter-reference Recency Set (LIRS) caching algorithm. This algorithm, and its approximation, have been widely adopted in major software products, including BSD and Linux operating systems, MySQL and H2 databases, Infinispan distributed systems, and other production systems.

Although LIRS may seem more complicated than the traditional LRU algorithm, it is a particularly effective method for data management in databases, operating systems, and data centres, because rather than just looking at when a specific page was accessed, it considers its reuse in a time interval, which is called ‘reuse distance’. Pages with short reuse distance are cached, improving the likelihood of caching the most useful data for improving performance.



Big Data Processing

'Big data' has been one of the most rapidly growing areas in society over recent years. Big data refers to such large and complex data sets that conventional data analysis tools simply cannot deal with them. However, despite these challenges, there has been such an explosion of interest in this field as it can offer important insights into a whole range of fields, including healthcare issues in the population and even predicting electoral outcomes.

Whereas standard PC hard drives often have around 1 Terabyte of storage space, this type of data set can be in excess of hundreds of terabytes. However, it is not just storing large volumes of data that poses a significant challenge – in order for this data to truly be useful, it needs to be rapidly accessible for analysis.

Conventional databases often store data in either a row or column store format. Row-store format has the advantage of being faster to load and includes a 'complete' dataset by rows in memory for analysis. However, not all the data elements in a row are used in practice, causing inefficient usage of limited storage bandwidth. Column-store means that any unnecessary or redundant data is not read into memory, but does not offer the same advantage of being a 'complete' data set. In addition, operations among distributed columns in different nodes require network communications.

Professor Zhang, in collaboration with research scientist Rubao Lee, former PhD students Yin Huai (now working at DataBricks) and Yuan Yuan (now working at Google), and several Facebook software engineers have designed and implemented a new type of data structure called Record Columnar File (RCFile) and its optimised version (ORC) that allows significantly faster memory access. With this hybrid structure containing both columns and rows, RCFIle and ORC retain the merits of both column-store and row-store methods, but minimise their limits. This has become the standard data storage format for large scale data processing systems, such as Hive (Hortenworks), Presto (Facebook), and Impala (Cloudera), but has also been adopted by major database vendors of IBM, Microsoft, Oracle, SAS, and Teradata for their commercial database products.

Algorithm Drives for Image and Graphics Processing

Generating computer graphics is typically one of the most demanding computational operations. When you are playing a video game, what you are actually seeing is shapes made up of polygons, rendered in different colours. As graphics have become increasingly realistic over the years, this means far higher polygon counts, which means more data to process and keep in memory.

Now, there is a great deal of interest in being able to visually represent the large datasets typical of the big data era. This makes use of the same polygon building blocks that make up video game graphics, but the size and complexity of what needs to be visualised often means that several layers of these polygons need to be used to reconstruct things like 3-D maps or automate diagnosis of medical conditions from images or scan data.

While graphical processing units (GPUs) are optimised for dealing with these types of processes, Professor Zhang, alongside former PhD students Kaibo Wang (now working at Google), Yin Huai, research scientist Rubao Lee, and two faculty members in Emory University, have found an algorithmic approach to greatly speed up these complex polygon overlay operations. This algorithm is known as PixelBox and has been adopted in the Geometric Performance Primitives (GPP) Library – an industry-leading and high speed computational geometry engine. GPP has also been included in the GPU-Accelerated libraries of the NVIDIA Company.

Future Directions

With data sets becoming ever larger, building powerful supercomputers for analysis is no longer an effective and affordable answer. Much of Professor Zhang's recent work involves 'distributed computing'. Rather than having one solitary powerful computer to run a big task, in a distributed computing arrangement, this task is split over multiple computers so the workload is shared and it is completed more efficiently in a cost-effective way.

However, there are significantly more memory management issues and other hardware challenges due to the rapid advancement of high performance devices, such as Graphics Processing Unit (GPU), Field-Programmable Gate Array (FPGA), Solid State Devices (SSD), and Non-Volatile Memory (NVM), when dealing with an entire network of computers rather than just one, and there is a need to design algorithms that exploit the unique capabilities of running distributed computing. Professor Zhang, alongside his group at The Ohio State University, will continue to spearhead the development of new algorithms and of an inclusive software environment for heterogeneous hardware devices to ensure this happens.

Meet the researcher

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Professor Xiaodong Zhang graduated with a PhD in Computer Science from University of Colorado at Boulder, where he received a Distinguished Engineering Alumni Award in 2011. He is currently the Robert M. Critchfield Professor in Engineering and Chair of the Computer Science and Engineering Department at The Ohio State University. Professor Zhang has made significant contributions to the fields of computer memory systems and data and memory management in distributed systems, for which he was named as IEEE Fellow (Institute of Electronics and Electrical Engineers) in 2009 and ACM Fellow (Association for Computing Machinery) in 2012. His research focus has been on finding ways to translate basic computer science research into high-impact technologies, and much of this work has been contributed to the public domain through open-source software and published papers.

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SEARCHING FOR THE PERFECT PICTURE

Currently, searching for images and videos on the Internet is less than ideal, with searches often providing completely irrelevant results. **Dr Gerald Friedland, Jaeyoung Choi** and their team at the International Computer Science Institute in Berkeley are working to develop better tools for image and video-based searches, to help researchers extract much more useful information.

Success in the current environment is increasingly dependent on Internet access – we find our jobs online, we pay our bills online, we identify that strange problem with our washing machine using information posted online. The Internet provides a vast sea of information about every topic imaginable – we can spend days learning about anything from auto repair to ancient Greece, from the history of zebra crossings to the health benefits of Zinc.

Yet all of this information is useless if we cannot find what we are looking for – the person looking for instructions to repair her car will be immensely irritated if all she can find are webpages about zebras. Thus, the ability to search and index online information is a necessity, and being able to do this efficiently and accurately has made search engines such as Yahoo and Google into multi-billion dollar corporations.

The complexity of the task means that search engines moved away from simple word matching long ago. Instead, the majority now balance information drawn from multiple sources – not only the text of the entire site being indexed but also the quality of other sites that link to it, and even the location and search history of the person typing the query. The outcome of this is that online searching is immensely more effective than it was a mere decade ago – to the point where we take relevant results for granted.

Part of this rapid increase in search relevance is due to the medium itself – the majority of the Internet is made up of text: words, sentences and paragraphs, just like this article. Text is very useful for computer analysis because it is relatively straightforward – it follows a well-organised set of rules (which we call 'grammar') and the meaning is relatively independent of the appearance (an 'a' is an 'a' regardless of whether it is written in Times New Roman or Comic Sans). This meant that search engine companies and their respective experts could focus on programming software to understand the meaning of text without worrying too much about extraneous problems.

Now, however, the Internet is rapidly filling up with visual media – there are hundreds of videos uploaded to YouTube every minute, and over one hundred pictures appear on Flickr in the same amount of time. A huge amount of information is now available in the form of film and images, yet it is exceptionally difficult to categorise.

This difficulty is predominantly due to the complexity of visual media – there is no 'grammar' for images, and no requirement that certain parts of the image be located and related in certain ways. Similarly, the same object can look very different in different images – a tree from the top and the side look completely unrelated, yet it is the same thing. This is not a problem for human viewers, as we excel in making conclusions based on limited data, but it is a nightmare for software systems.

The usual workaround for problems such as these falls under the lump term of 'big data' and 'machine learning'. Software can be written such that it will flexibly judge different pieces of a large data set, deciding for itself how to balance out the competing information. By 'training' the software on large amounts of known data, it will essentially write its own rules to analyse unknown data – rules that are often completely unlike those a human programmer would think of.

Machine learning approaches allow complex and ambiguous problems to be solved with ease, provided that there is sufficient data available at the beginning to train the system. They are, naturally, being employed in the field of image search.

‘A couple years ago, I had the dream that everybody should be able to do empirical studies using YouTube videos. Instead of travelling, like for example Darwin, everybody can just sit at home and collect real-world data out of videos.’ – Dr Friedland

Rounding Up Data

Thus, the development of an efficient image search program requires two main things – it needs clever engineers and scientists to program the software, and it needs a lot of images and videos to train the software. The SMASH program, led by Dr Gerald Friedland and Jaeyoung Choi at the International Computer Science Institute, sets out to provide both of these requirements by helping industry giants and computer science students to team up.

Both researchers have long experience in the field of computer science studies, and were particularly interested by the potential for using the large data sets provided by online image and video-sharing sites. ‘A couple of years ago, I had the dream that everybody should be able to do empirical studies using YouTube videos,’ says Dr Friedland. ‘Instead of travelling around the world, like, for example Darwin, everybody can just sit at home and collect real-world data out of videos.’

This was, however, very difficult. YouTube videos are searchable using categories and keywords, both text-based functions, and both reliant on the uploader including enough accurate information to make a correct assessment of the video content. This is possible in principle, but is not very reliable in practice. ‘The problem is, YouTube and the like don’t really allow searching for videos with the accuracy required for scientific research,’ explains Dr Friedland. ‘For example, while there are tens of millions of cat videos, just try to find cats with a certain attribute doing a certain thing. So “white cat deaf” only results in ONE relevant video to the topic and one lecture that explains the scientific correlation between white blue eyes and deafness in cats. In other words, we need much better tools for search.’

Developing these tools required developing the right set of data to work with, and this is where Dr Friedland and Choi began to work on what would eventually be known as the Multimedia Commons project.

Multimedia Commons

To improve research in the field of image and video, Dr Friedland, Choi and their colleagues formed a group called Multimedia Commons. Through this initiative, the team is heavily involved in improving a publicly available dataset known as the Yahoo-Flickr Creative Commons 100 Million dataset, usually referred to as YFCC100M for simplicity. This dataset contains the metadata of about 99.2 million photos and 800 thousand videos – details on where the image was taken, who took it, what camera was used, etc. Although this is useful, the dataset does not contain any of the actual images themselves, which excludes those researchers who are interested in extracting information from the image itself rather than the metadata.

To make the information more useful, the Multimedia Commons program has collaborated with Yahoo to provide all of the original images and videos. This improved dataset has then been enhanced by adding further information, such as visual features, image information, and other annotations. The enhanced dataset has already been used in several different ways by organisations affiliated with the SMASH/Multimedia Commons groups.

One of these uses is known as the MediaEval Placing Task – a competition organised by the team in which contestants must develop software that can estimate where a photo has been taken, based on the content of

the image and the additional data. Each contestant is provided with 5 million photos to help train their machine learning software, they are then graded on the identification of a set of 1.5 million images. This competition helps to develop the next wave of image recognition and search software, bringing together multiple different approaches with a common goal. Competitions of this sort also lead to various entertaining discoveries, such as Dr Friedland's recent finding that the ability to locate a photo can be reduced through the use of simple Instagram filters – a definite plus for those worried about the privacy of the photos that they upload to the Internet.

Data Analysis

Working through and analysing thousands of images requires slightly more power than the average home computer or laptop can provide. To speed up their work, many researchers in the field of machine learning rent computer time from a central server farm as they need it. This idea is actually quite old (having been behind the terminal/mainframe approaches of the first computers) but has been reborn under the term 'cloud computing' – researchers do not need to own a blindingly fast computer, they just need to rent it from someone who does.

One of the biggest companies in the cloud computing space is Amazon, who provide processing time to companies and institutions through their Amazon Web Services subsidiary. This subsidiary has grown from a small start-up into a billion-dollar business used around the world. Amazon Web Services is currently collaborating with the SMASH/Multimedia Commons group to provide free hosting of the vast amounts of data required by the scientists. This can be downloaded for free if required, but many researchers choose to use cloud-based streaming and storage processes to allow them to access only the required data as they go. This saves on download bandwidth and storage space (as 100 million pictures take up quite a few hard drives) and speeds up the process of analysing the data significantly.

Dr Friedland, Choi and the team have further simplified life for their collaborators by developing a series of software tools which would allow the dataset to be analysed. 'We built tools which allowed simple interfacing between Jupyter Notebook, a beginner's data science tool, and image search in the cloud,' says Dr Friedland. 'An example tool allows you to predict the location in which an image was taken based on the similarity to other images.' These tools are designed to be launched easily on Amazon Web Services, and so can be used in combination with Amazon's existing machine learning framework and infrastructure. This essentially allows even the worst-equipped computer scientist to develop their own multimedia search programs.

The Future of Search

The amount of information available to us is currently increasing at an astonishing rate – news articles, books, pictures and videos are appearing online every millisecond. Yet none of this is useful if we cannot identify the information we need amongst the vast sea of irrelevant results. In particular, the current status of image and video-based searches is less than ideal – results are often obscure or not related to the subject at hand. The work of groups such as Multimedia Commons are thus vital in providing the groundwork for these image searches, essentially setting up the laboratory in which these new discoveries will be made.

Perhaps, one day, you will be able to confidently ask your computer to find that picture of your Aunt Gladys by the pool in summer 2017 – and be confident that you will get the correct picture back. When that day arrives, it will be in no small part due to the actions of researchers such as Dr Gerald Friedland and Jaeyoung Choi.

Meet the researchers

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Dr Gerald Friedland's research career has stretched across the globe, having begun with a PhD from the Freie Universität Berlin in Germany and progressing over his role as Director of the Audio and Multimedia lab at the International Computer Science Institute to his current role as the Principal Data Scientist at Lawrence Livermore National labs. He is also an adjunct faculty member at the EECS department of the University of California, Berkeley. With over 200 published articles in conferences, journals, and books, and recipient of a number of awards, Dr Friedland is a leader in the field of multimedia search and processing.

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Jaeyoung Choi is currently a staff researcher at the Audio and Multimedia lab of the International Computer Science Institute in Berkeley, California. Much of his research to date has focused on the extraction of useful information from multimedia and in the management of online privacy due to image and information sharing. His years of working on this topic have led to a number of publications and awards. He is currently also conducting research towards attainment of a PhD degree from Delft University of Technology in the Netherlands.

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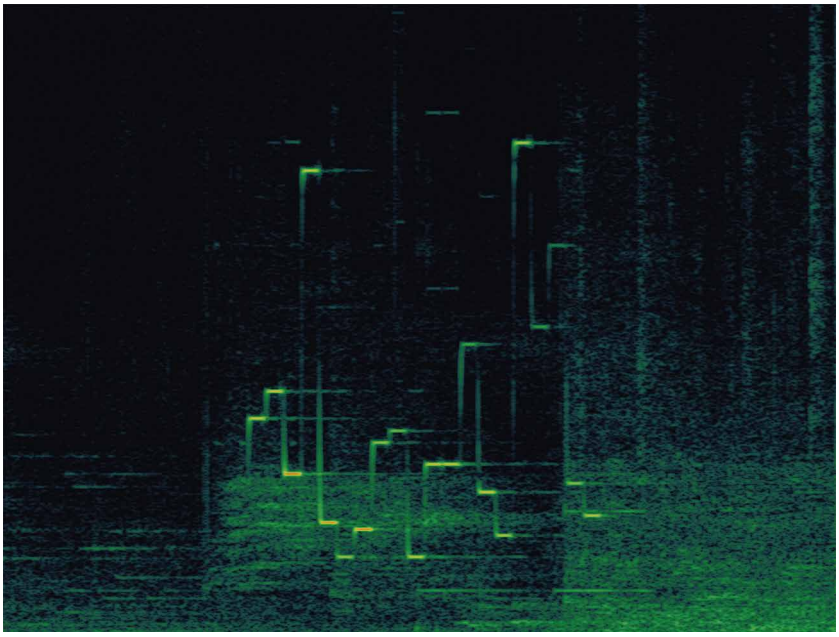
FUNDING

This work was graciously supported by AWS Programs for Research and Education. We also thank the AWS Public Dataset program for hosting the Multimedia Commons dataset for public use. Our work is also partially supported by a collaborative LDRD led by Lawrence Livermore National Laboratory (U.S. Dept. of Energy contract DE-AC52-07NA27344) and by National Science Foundation Grant No. CNS 1514509.

CHIRPING COMMUNICATION – SENDING DATA OVER SOUND

Dr Daniel Jones, Chief Science Officer of Chirp, and his colleagues have developed a technology that enables fast, effortless and cheap data transfer using the power of sound waves. Chirp's data-over-sound technology has been used in numerous applications for wireless communication, spanning sectors from children's games to industrial powerplants.



Spectrogram showing the frequency content of a chirp

Vibrating objects generate sound waves that can travel through gas, liquid and solid mediums. Actions that generate sound energy, such as ringing a bell, cause particles in the air to vibrate, resulting in small fluctuations in air pressure. These air pressure fluctuations propagate, as the vibrating air particles collide with neighbouring particles, which then also start vibrating. Collectively, this travelling disturbance in air pressure and particle vibration is referred to as a sound wave. When sound waves reach the ear, they cause the eardrum to vibrate, initiating a neural impulse that is interpreted by the brain as sound.

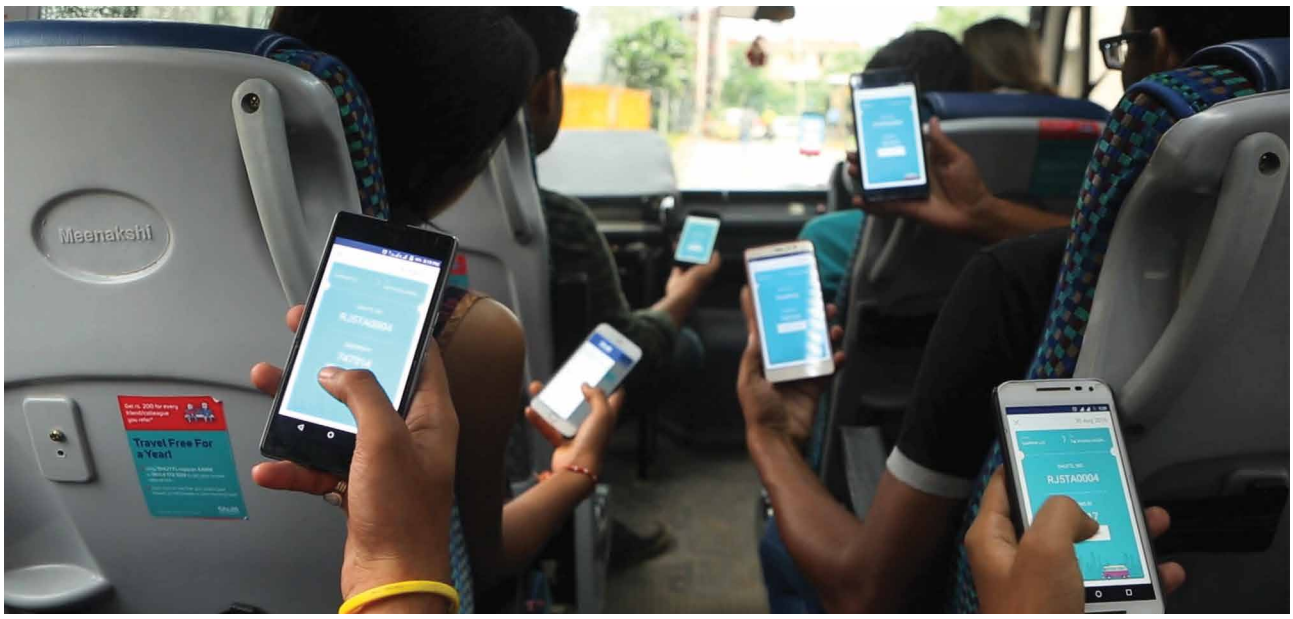
Sound waves always require a medium to travel through, and thus cannot propagate in a vacuum. One important property of a sound wave is its frequency, which describes how quickly the wave's air particles are vibrating. Higher frequency sound waves, which cause the air particles to vibrate faster, are picked up by our ears as higher pitched sounds – if within the audible range of frequencies that can be detected by the human ear.

When it comes to transmitting data between devices, the traditional choice is radio waves –a type of electromagnetic radiation, along with visible light, x-rays, microwaves, etc. Rather than involving vibrating gaseous, liquid or solid particles, electromagnetic radiation can be described as electric and magnetic fields vibrating together in space. Wi-Fi and Bluetooth both operate through radio waves, and in order to use these technologies, devices must contain chips that can transmit and receive radio frequencies. Such devices are referred to as 'enabled' for Wi-Fi and Bluetooth, and their use can often be difficult due to the setup and pairing processes required.

Because Chirp uses sound waves rather than radio waves, the technology offers a convenient approach to transferring data, and can be integrated into many existing devices, as it only requires a speaker in the sending device, along with a microphone and a small amount of processing power in the receiving device. Chirp's technology offers many advantages over Wi-Fi and Bluetooth, as the setup and pairing processes are removed, and sound can be immediately broadcast to nearby receiving devices. Additionally, sound offers the benefits of geographical co-location: if a user can hear a device 'chirping', then they must be nearby to it, making it easy to establish that the person with the sending device is in the same room. This can be used, for example, to only allow hotel guests to sign on to the Wi-Fi with a Chirp, by virtue of the fact that only they have access to their own room.

The team at Chirp developed this technology to facilitate communication between devices of different platforms, form-factors, architectures and eras that run on completely different operating systems and may or may not be connected to a network, thereby fulfilling a niche area in the data communications market. Sound can also travel through other media; for example, P.A. systems in commercial buildings, radio broadcasts, or even websites and feature phones.

‘Using sound has been a powerful way of communicating data since the earliest days of telecommunications, from telegraphs and Morse code to dial-up modems. The difference is that we have developed algorithms that work “over the air”, in noisy and acoustically challenging environments.’



Developing Chirp – From Concept to Commercialisation

The concept of using sound to relay a message between two devices is not unique to Chirp’s data-over-sound technology. ‘Using sound has been a powerful way of communicating data since the earliest days of telecommunications, from telegraphs and Morse code to dial-up modems,’ says Dr Daniel Jones, Chief Science Officer of Chirp. The unique aspect of Chirp’s technology is the use of algorithms that enable data to be sent between spatially-separated devices, using consumer-grade speakers and microphones, in noisy, real-world environments, over the air.

The first experiment that kick-started the development of Chirp’s technology was carried out in 2011 in the Computer Science labs of University College London, UK. The research team showed that data sent over sound waves could be successfully received by mobile phones that had even been placed under heavy mattresses in a noisy environment. Chirp initially launched the technology to market as a consumer facing iOS and Android application that enabled peer to peer content sharing. Although popular, particularly in the education sector where teachers could share content and links to an entire class with the press of a button, Chirp took the decision to repackage the technology into a suite of cross-platform Software Development Kits (SDKs), making it available for other companies to build into their own technology products.

Since this initial experiment and the repackaging of the software into cross platform SDKs, Chirp’s technology has grown into a widely adopted, versatile, convenient, simple and reliable method for wireless communication, which can rapidly send and receive data. The technology excels in areas of low internet coverage, or within dead spots of network coverage in industrial locations. Furthermore, Chirp’s software can be easily and inexpensively integrated into existing infrastructure, and does not require extra networking modems or signal amplification points to be installed. Chirp is now a global leader in data-over-sound communication capable of transmitting data over distances of more than 30 metres, and in regions of extreme background noise. ‘Our first consumer app was used by hundreds of thousands of people worldwide, in offices, bars, cafes and nightclubs,’ says Dr Jones, highlighting the diversity and flexibility of this technology.

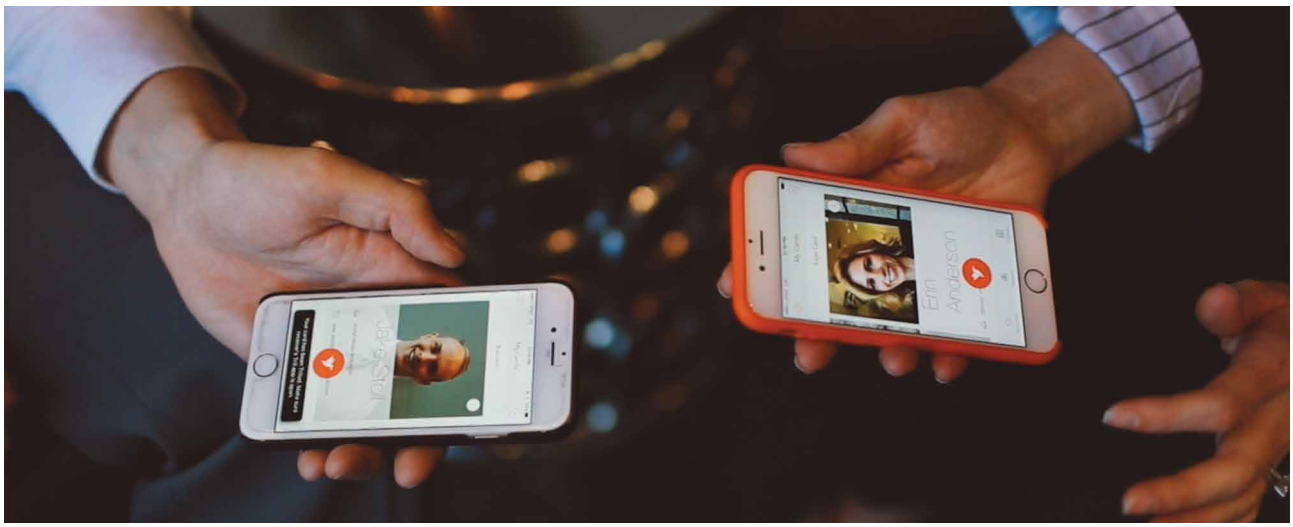
The Chirp team, comprising leading scientific and engineering researchers, has been continuously improving Chirp’s data-over-sound technology, thus accelerating of the software from a simple start-up idea to an established global technology.

How Can Chirping Sounds Carry Data?

The key functionality of Chirp’s technology is that it uses algorithms that convert data at a transmitting device into a series of whole numbers (called integers) through a process called ‘modulation’. The values of these integer numbers determine the frequency (or pitch) of a sound wave that the device will generate. First, Chirp’s software translates a message into an array of integer numbers, and then it creates a ‘tune’ or pattern, which is made up of many sounds, each with a different pitch. This tune is then emitted from the transmitting device and the data is carried through the air.

The receiving device with Chirp’s SDK installed detects the incoming sound wave and measures the different pitches of each sound in the tune. This combination of sound pitches is converted back into the original array of integer numbers by a process called ‘demodulation’. Thus, the original message is transmitted to the receiving device, and relayed to the application via the Chirp SDK.

The modulation of messages allows data to be encoded into what could be described as a ‘sonic barcode’ that can be transmitted between devices. Although other methods for encoding data in audio exist, the use of modulation/demodulation gives Chirp’s technology several advantages. Firstly,



modulation/demodulation generates a new signal for each new set of data and does not require an existing audio signal to operate on. Also, the process of modulation does not need an external database to look up the data, allowing datasets to be transmitted offline with no time delay.

Worldwide Applications of Chirp's Software

Chirp's SDKs have been installed on millions of devices worldwide, used across a broad range of applications. These applications include children's toys, virtual reality technologies, industrial machinery controls and transport.

Chirp has recently announced their collaboration with Hijinx to create toys that magically interact with content on any device. This partnership launched with the official Hijinx Alive™ Powered by Chirp Interactive Beat Bugs toys, to accompany the Emmy-award winning Netflix TV series, where episodes explore the narratives of songs by the Beatles in a child-friendly fashion. Instead of embedding 'Chirps' into pre-existing television audio (due to the risk of streaming platform compression methods stripping these out), Chirp created a new technology for this partnership. In this new technology, the toys themselves recognise portions of the show's audio, and this triggers a specific action for the toy. For Beat Bugs, the toys sing in sync with their counterpart on-screen characters, reacting within milliseconds of hearing the audio.

Another significant area where Chirp's software has been successfully applied is within the transportation sector. Since mid 2016, a mobile app running Chirp's software has been used to authenticate passengers boarding buses in India. The transportation company, called Shuttl, provide shuttles between different locations in the city of New Delhi, India. With a population of over 27 million people, public transport in New Delhi is famously chaotic, and the increased number of cars on the road has added to congestion and pollution. Thus, Shuttl saw challenge that needed to be addressed. Shuttl uses Chirp's software to allow passengers to transmit messages to a device held by the driver. This message is unique to each user and so can be used to identify each passenger. 'The technology has significantly reduced the workload of their drivers, and has successfully become incorporated into their existing infrastructure,' states Shuttl's director.

Kawa Coffee is a specialist coffee shop chain operating in Hong Kong and China. The coffee shop staff wanted a compact and secure device that would enable customers to pre-pay for coffee and then redeem their purchase in store. To meet these requirements, the 'Kawa Box' was developed – a technology that can operate without an internet connection or screen. The simple and elegant wooden box encapsulates a device that simply plays out wav files, each representing different price points dependent on the coffee ordered. When a customer's device with the Kawa app installed is held over the Kawa Box, the box plays the appropriate wav file and the coffee purchase is redeemed within the app. The Kawa box is unlike any other non-contact payment methods, which are often expensive and require bulky equipment and an active internet connection. Chirp's software has enabled the Kawa Box to be a portable and scalable solution for in-store redemption.

Although the team behind Chirp's technology is modest, their product is powerful and versatile, and its current applications highlight the diverse potential of the technology.

The Future for Chirp's Data-Over-Sound Technology

As a company, Chirp's future ambition is to continue to enable communication routes between millions of people and devices, across a broad range of applications, making data transmission between devices seamless, scalable and cost effective. Dr Jones has a vision of enabling any device to connect, interact, and share data with another by focusing on continuous research and development. 'I think Chirp is a powerful and frictionless way of pairing two devices,' he states. 'More than anything, we're thrilled to see the imaginative ways in which our partners have harnessed the power of Chirp.'

Meet the researcher

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Dr Daniel Jones directs Chirp's R&D programme, leading research into the next generation of acoustic communication technologies. He has been involved in developing Chirp's technology since the first proof-of-concept experiment in 2011, in which the underlying engine that powers Chirp's technology was developed.

Dr Jones graduated with a PhD from Goldsmiths, University of London in 2015, for a project that applied high-performance computing to evolutionary simulations. His other research projects have included Phantom Terrains, a mobile framework that allows hearing-impaired users to hear Wi-Fi signals, and Maelstrom, which uses audio material from media-publishing websites as a distributed, virtual orchestra. Dr Jones developed the innovative 3D audio engine for the BAFTA-nominated mobile games Papa Sangre and The Nightjar. He was also a fellow on the Mozilla Webmaker programme.

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CAPTIVE: A NEW DIRECTION FOR VIRTUAL REALITY CONTROLLERS

Virtual and augmented reality systems are transforming how we view and manipulate 3D objects. One of the biggest challenges to developers is to design fast, accurate, yet affordable controllers. Now, **Professor Christopher Healey** and **Zeyuan Chen** at North Carolina State University have announced the creation of CAPTIVE – a controller system they believe will do just that.

One of the most important elements in virtual and augmented reality systems is their controller. As an architect or a doctor, you may wish to accurately inspect complex 3D objects from every angle. If you play video games, you want your in-game character to perform fluid, realistic movements through virtual worlds. Images that lag noticeably and don't accurately reflect how you manipulate the controller can be frustrating and disorientating, making the systems difficult to use.

When deciding on a controller for a virtual/augmented reality headset, you may be faced with a trade-off. A 3D mouse like 3Dconnexion's SpaceNavigator may be your first choice – with its pressure sensitive handle, it is a fairly simple, cheap option, but is difficult to control. Like flying a kite, any sleight of your hand could send your image careering off in the wrong direction, and you could spend hours learning to control the device properly. On the other end, free-moving devices like the HTC Vive are much easier to learn to control, but their complex arrangements of sensors and base systems make them much more expensive.

Recent developments have brought about desirable alternatives – systems such as MagicMouse and ARToolKit use a single camera to track 2D marks on a physical controller. These systems are simple, cheap and easy to control, but their tracking algorithms have a long way to go. Transitions between frames of moving augmented reality images can be clunky and inaccurate, making the experience disorientating to users. Changes in lighting and objects in the background can also make it hard for the system to detect where the controller even is, which could render the system unusable.

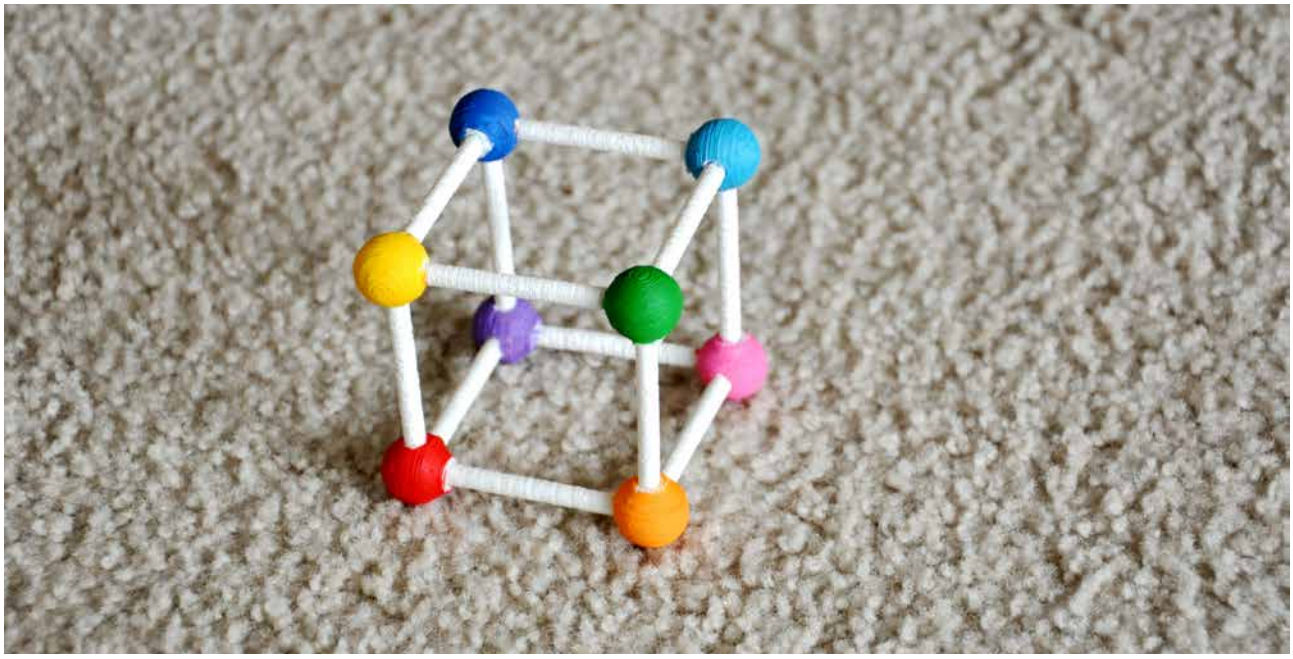
Professor Christopher Healey and Zeyuan Chen at North Carolina State's Department of Computer Science have created a system they believe will be cheap, easy to control, and functional in many lighting environments, all while operating at 63 frames per second (https://youtu.be/gRN5bYtYe3M). 'Our system consists of a 3D-printed wireframe cube, a regular RGB camera and our program,' explains Chen.

Tracking Movements

When you move a computer mouse, two primary motions, or 'degrees of freedom' affect the position of the cursor on the screen: forwards/backwards and left/right. Professor Healey and Chen's controller has a much more varied range of motion. As well as those two initial degrees of freedom, their software detects when the user is moving the cube up or down, or rotating it about all three axes (motions called yaw, pitch and roll). This brings the number of degrees of freedom up to six – reflecting any possible way you could move a rigid cube through space.

The first step that CAPTIVE's software takes is to map out a rough region containing the cube within each frame the camera captures. Using previous frames, and the system's knowledge of the shape of the cube, it can change the shape and location of the region based on previous trends in the cube's motion. It uses

‘The primary advantage of CAPTIVE is that it is efficient. There are a number of tools on the market that can be used to manipulate 3-D virtual objects, but CAPTIVE allows users to perform these tasks much more quickly.’



these trends to predict where the region should be in the next frame, ensuring smooth transitions between frames. At 63 frames per second, ‘there’s basically no latency, no detectable lag time between what the user is doing and what they see on screen,’ says Chen.

The next task is to detect the exact pose of the cube within the region. CAPTIVE does this using the eight uniquely-coloured balls that comprise the eight corners of the cube. Within the rough region in each frame, the software locates the positions of each corner of the cube. It then compares these positions with a virtual cube stored in the software.

Like the physical cube, this virtual image has a different colour assigned to each of its corners, meaning that you can always tell what angle you are viewing it from, based on the orientation of its corners. The size of the virtual cube is defined by a 3D coordinate system, with its origin located at the centre, and each corner positioned at a unique coordinate.

By aligning the images of the real cube and the virtual cube, CAPTIVE calculates the exact pose of the real cube in physical space and establishes a new coordinate system in each frame. Each new coordinate system acts as a canvas on which the frames of virtual reality objects are projected. Because new coordinates are established in each frame, the user will see 3D objects with movements that reflect how they move the cube in real life. Like the cube, these objects will also possess six degrees of freedom, meaning users can manipulate them in any way they wish.

The researchers also designed innovated methods to use CAPTIVE as a joystick-like controller by mapping the calculated 3D information to velocity of virtual objects. Because CAPTIVE’s cube is free-moving, it doesn’t have a ‘default’ position like most controllers. This means that, in the ‘joystick’ mode, when the user moves the cube, the 3D object will carry on moving when the cube stops, based on the trends in motion that the tracking software picks up. To stop the object from moving, bringing it back to a ‘neutral’ position, the research team has implemented a ‘pedal’, which the user can press any time they want.

‘The primary advantage of CAPTIVE is that it is efficient,’ Chen explains. ‘There are a number of tools on the market that can be used to manipulate 3-D virtual objects, but CAPTIVE allows users to perform these tasks much more quickly.’

Imperfect Lighting and Noisy Environments

Professor Healey and Chen's tracking system is simple but effective, yet the combined task of CAPTIVE's camera and its software isn't so easy. In practical use, different lighting environments can significantly change the colours of the eight corners as they appear to the camera, and other objects in the background can clutter the image, making it harder for the software to pick out the cube's position. These issues have caused problems for previous controllers, but the researchers believe they have found solutions in their software.

To combat the challenges posed by unpredictable lighting, the team has made use of Hue, Saturation and Value (HSV) colour space. HSV space consists of a colour wheel in which colours fade into each other, with darker shades around the edge fading to white towards the centre. In different lighting environments, the colours of the cube's corners will appear to vary, corresponding to different positions in HSV space. So rather than picking up single colours, the software is programmed to detect a corner if its colour appears in a particular small region of HSV space. Thanks to this approach, users don't need to worry about the CAPTIVE becoming unresponsive when lighting conditions change.

Virtual reality systems can also become confused when their cameras pick up objects other than the controller, but the software can deal with this too. If it is initially confused by background clutter, it can recognise when pixels in the frames fall inside circle-like regions, as the balls comprising the cube's corners, appear to the camera. If any pixel doesn't meet these criteria, it is blocked out, making only the cube's corners visible to the software. So instead of needing to set up the system in a sterilised lab environment, users can use CAPTIVE in more practical settings.

Practical Uses

CAPTIVE could offer enormous benefits to fields including medicine, architecture, archaeology and geology, to name just a few. By simply integrating CAPTIVE into other stereo systems, users can project their models and 3D objects onto the cube as augmented reality images. They can literally hold projections in their hand, and easily and accurately inspect them from any angle. Furthermore, the system could be set up in locations ranging from operating theatres to remote wildernesses, making it much more practical than other devices. With further improvements, users could even use tools like a stylus to directly interact with and manipulate the images.

Video game creators have also begun to invest heavily in the technology, but various controller-related difficulties have prevented any titles from becoming hugely popular so far. Motions including rotation have been difficult to translate from the user's hand to the virtual world, often making movements slow and disorientating. CAPTIVE's six degrees of freedom could solve this issue, enabling players to move and rotate objects fluidly and realistically. The use of the technology as a joystick controller was the subject of an experiment the researchers carried out themselves.

Experimenting with Real Users

Chen, Professor Healey and their colleagues tested CAPTIVE's usability with the help of 15 of North Carolina State's computer science graduate students. Projecting a virtual reality image of a house inside the cube, they asked the participants to rotate the house to a target position as quickly and accurately as possible. They essentially used the cube as an input device. But unlike similar previous tests, the participants' view was affected by their head movements, which added an extra layer of difficulty to the task. The researchers were confident that CAPTIVE's ease of control, and rapid frame rate, would offset this difficulty.

On average, the students completed the task in just 2.79 seconds and missed out on a perfect rotation by an angle of 6.2 degrees. The results were a drastic improvement on experiments with similar controllers, with participants completing rotations almost twice as fast. They almost matched the performance of a much more complex and expensive system, known as a surround screen virtual environment, though they were not quite as accurate.

Despite the experiment's success, not everything went perfectly. Strangely, three students had difficulty in mentally connecting the 3D image they saw with the cube they were holding. The researchers decided that more research would be needed to understand why the technology could be more cognitively difficult to grasp for certain people.

'We are improving the accuracy and robustness of this tool, especially in outdoor environments, using deep learning methods,' Chen claims. 'Additionally, we are combining this tool with mobile devices (e.g. iPhones) and professional virtual and augmented reality devices (e.g. the Microsoft Hololens).' The team would also like to develop a cube with a more translucent wire frame. Augmented reality images can be disorientating to users when the cube's frame visibly passes in around their image. A less intrusive cube design is desirable but would require more work to implement. In the future, they would like CAPTIVE to project two separate frames for user's eyes to improve their depth perception, which would make 3D images more realistic. The technology still has a way to go, but for any virtual reality enthusiast, CAPTIVE is a truly exciting development.

Meet the researchers

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Professor Christopher G. Healey is a Professor in both the Department of Computer Science and the Institute for Advanced Analytics at North Carolina State University. He completed his PhD in computer graphics at the University of British Columbia in Vancouver and has since received $5.5 million in funding from both the government and industrial partners, for his world-leading research in computer science. Professor Healey's accomplishments have earned him the National Science Foundation's CAREER Early Faculty Development Award, and the Outstanding Instructor Award from North Carolina State University.

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Zeyuan Chen is currently completing his PhD in the Department of Computer Science at North Carolina State University, where his areas of research include visualisation, computer vision, and human-computer interaction. Prior to starting his PhD research, Chen studied Electronics and Information Engineering and Information Engineering at Huazhong University of Science and Technology in China, and then completed his Master's degree in Electrical Engineering at Cornell University. He has a keen interest in designing computer graphics, and a selection of his creations can be found on his website.

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FUNDING

US National Science Foundation

NC STATE UNIVERSITY

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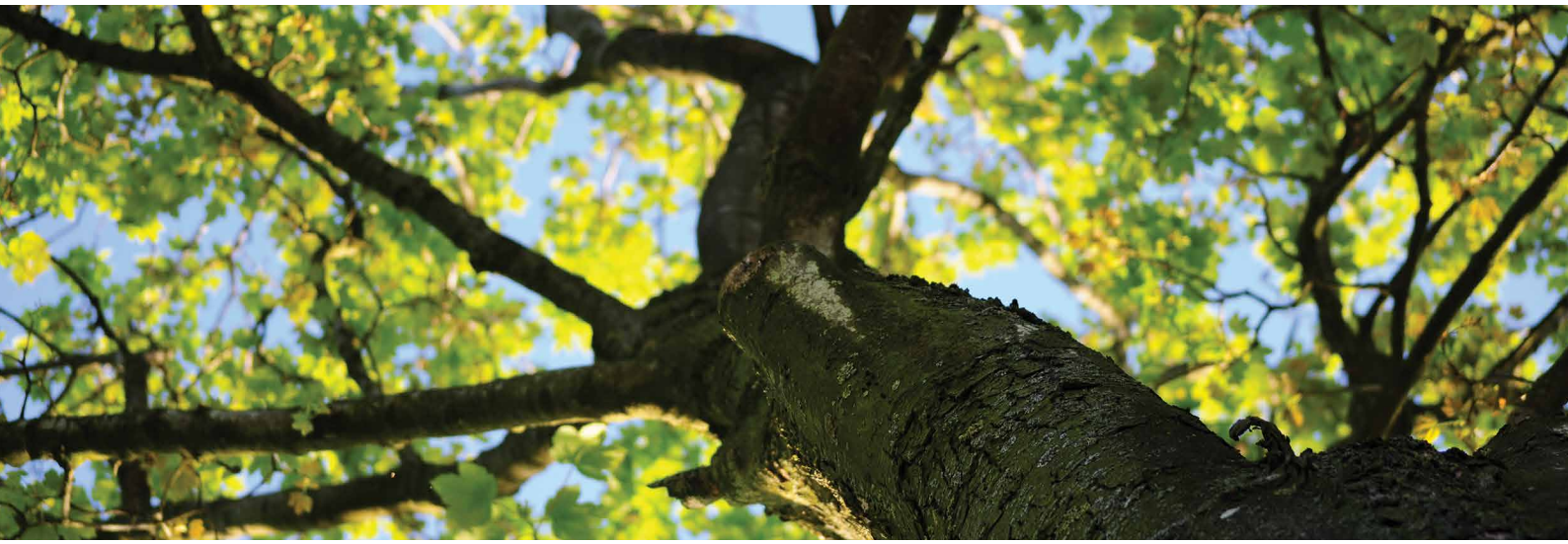

WHO WE ARE

Trees for Cities is the only charity working on an international scale to create greener cities. Since 1993, we have engaged over 70,000 people to plant over 650,000 urban trees in parks, streets, schools and housing estates across the UK, as well as internationally, revitalising these areas and improving the lives of the people who live in them. We strengthen communities through volunteering opportunities and inspire children to grow and eat good food and to connect with nature.

WHAT WE DO AND WHY WE DO IT

We focus on planting trees and greening community spaces where the social and environmental impact on local people is greatest. In London this might mean planting trees to clean the air or transforming unused community spaces into vibrant green areas, making our communities happier and healthier places to live, whilst in Nairobi it's planting fruit trees for food and sustainable livelihoods.

HELP US PLANT A MILLION URBAN TREES BY 2020

To date we have planted over 650,000 trees in cities. We have now set ourselves an ambitious new target to strive to plant 1 million urban trees by 2020. Help us meet this exciting new milestone...

CORPORATE PARTNERSHIPS AT
www.treesforcities.org/corporate-services/

DONATE ONLINE AT
www.treesforcities.org/donate/

FIND OUT HOW TO GET INVOLVED AT
www.treesforcities.org/get-involved/

MISSION

- Planting trees and greening cities worldwide.

VALUES

- **People-led:** Although our reach is global, we value the importance of a local focus. We always work through and within local communities to strengthen them and empower their members.
- **Quality-driven:** Both the quantity and quality of the trees we plant are at the forefront of our planning so that we constantly strive to maximise the impact of our projects to the environment and society.
- **Delivery-focused:** We are an organisation that gets things done. What we talk about, we do – effectively, efficiently and on-time.

WHY TREES MATTER

- Trees help our environment and the impact of climate change:
- They remove 4m tonnes of carbon from the UK atmosphere each year (Forestry Commission 2010)
- They can cool the air by 2 - 8 degrees C
- Trees absorb water , lowering stress on storm water drains and mitigating flood risk
- A single mature oak tree can host up to 423 different species of invertebrates that support birds and mammals
- Each year Trees for Cities plant around 65,000 trees in cities worldwide, revitalising cities and enhancing the lives of the people that live in them.