Scientia

QUANTUM LEAPS FOR PHYSICS AND ENGINEERING

HIGHLIGHTS:

- Manipulation of Molecular Quantum States
- A Novel Electric Current Simulator in the Human Brain
- Renewable Energy gets a Boost from Sodium Battery Technology
- Capturing the Forgotten Source of CO_2

Issue: #105

WELCOME...

There has never been a more exciting time for physical science and engineering. The last few years have witnessed some of the most ground breaking discoveries ever made, such as proving the existence of the Higgs boson, the elusive elementary particle that bestows other particles with mass. Even in the past year alone, scientists have made the first detection of gravitational waves, ripples in the fabric of space time first theorised by Albert Einstein a century ago. Then just a few months ago, the Hubble telescope astounded us by imaging the farthest galaxy ever observed, seen as it existed a whopping 13.2 billion years ago, when the photons captured by Hubble first began their journey. To celebrate these huge leaps for fundamental physics and astronomy, for the first section of this edition we have had the pleasure of interviewing representatives from Fermilab, the United States' premier particle physics laboratory, and The European Southern Observatory, the world's most productive ground based observatory, home to the Very Large Telescope (VLT).

Such fundamental advances in unravelling the nature of the universe have given rise to an abundance of new technologies. As we will show in our next section, understanding how matter works on a quantum level, for example, has advanced research in areas such as computing, telecommunications, GPS and medical technologies such as MRI. Here we highlight the work of Dr Hayakawa, who's research into the development of molecular devices holds the promise of dramatically reducing the size and increasing the speed of our computers. The quantum effects demonstrated by these devices may also lead to a completely new type of computing, known as quantum computing.

In our next section, we delve into the mathematics behind computer processing, where we showcase the work of Dr Kansa, pioneer of the Kansa method. From here, we show how mathematics and computing are applied to fields ranging from the development of automated systems for unmanned aircraft to the analysis of electromagnetic phenomena in the human body.

Our final section highlights the latest innovations in clean energy technology. Here we introduce three teams of researchers dedicated to generating clean power using nuclear fusion, storing energy efficiently using the latest battery technologies and capturing carbon dioxide to prevent its release into the atmosphere. In these challenging times of rising global temperatures and imminent environmental chaos, clean energy technologies are perhaps the most important application of physical science and engineering.

Science Diffusion

CONTACT

Science Diffusion ltd

Published in the UK, by
Science Diffusion ltd

E: info@sciencediffusion.com
W: www.sciencediffusion.com
W: www.scientiapublications.com

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

Meet The Team...

EDITOR-IN-CHIEF
Dr. Nelly Berg
nelly@sciencediffusion.com

PUBLICATION MANAGER
Nick Powers
npowers@sciencediffusion.com

DESIGN MANAGER
Mimi Jones

CONTRIBUTING WRITERS
Christopher Harrison, PhD
Alma Ionescu, BSc
Rafael Bernar, PhD
Edd Gent, BA

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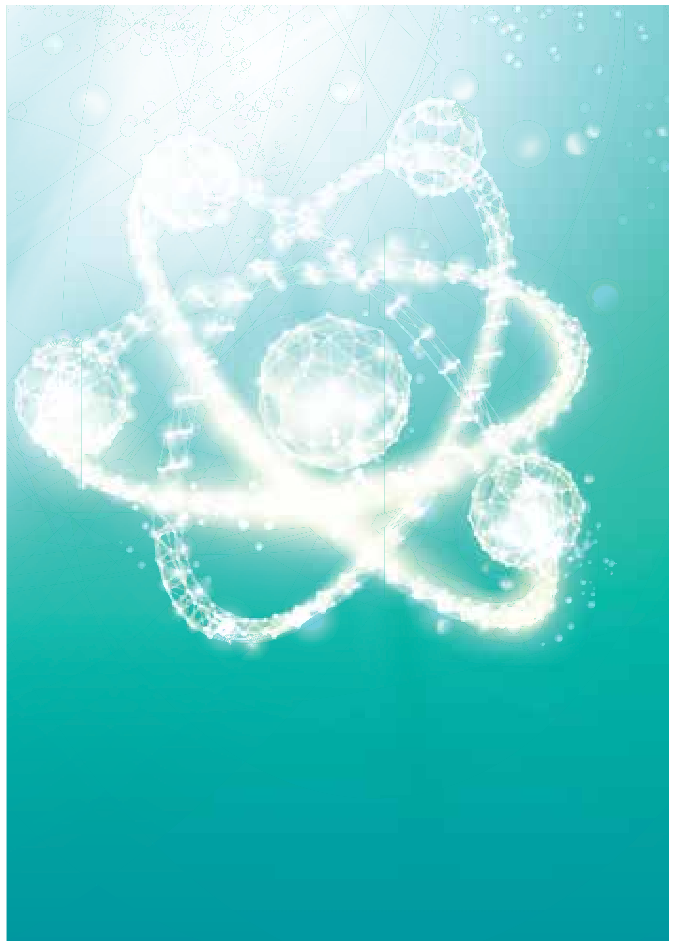
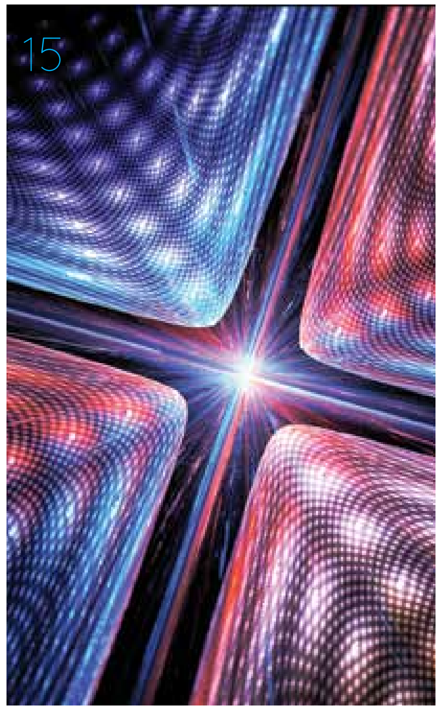
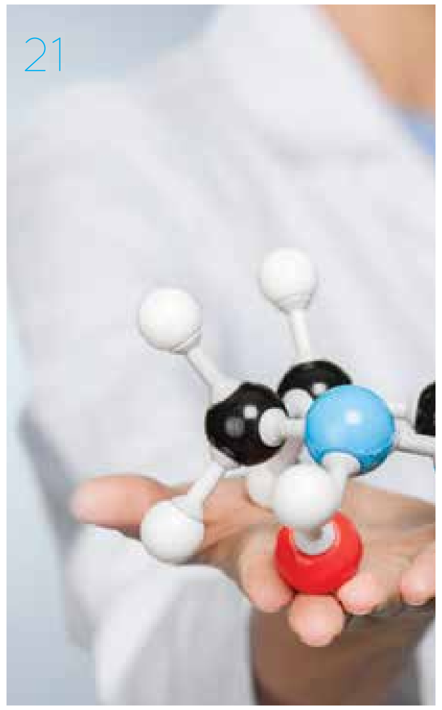


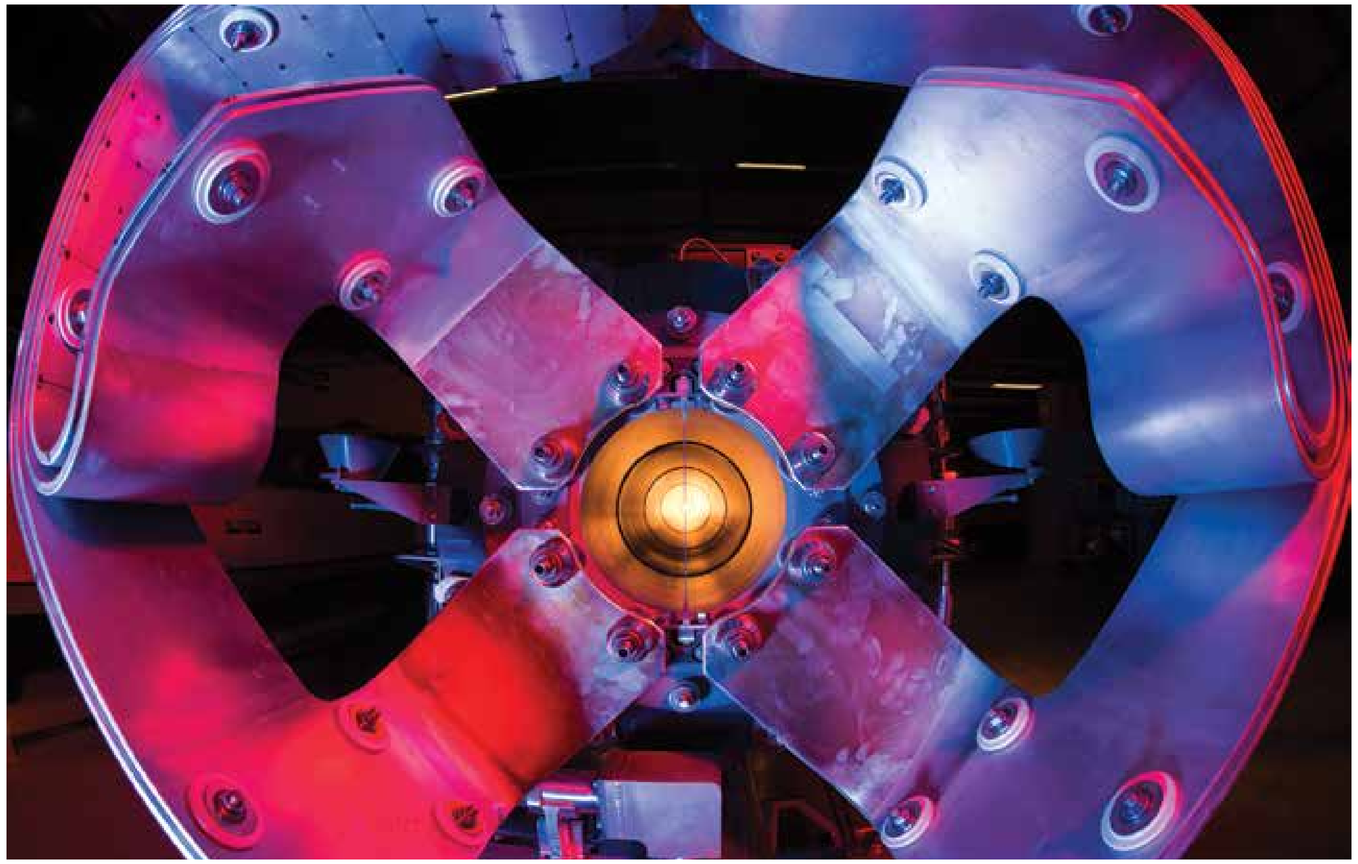




FERMILAB

Situated on a 6,800-acre site, home to a herd of bison and almost 300 species of bird, Fermi National Accelerator Laboratory (Fermilab) in Illinois has been working to enhance our understanding of the universe since 1967. From investigating the properties of the tiniest elemental particles to probing the nature of dark matter and dark energy in the farthest reaches of the universe, scientists and engineers at Fermilab are busy untangling the mysteries of our physical reality. Here we speak to **Dr Katie Yurkewicz,** who tells us all about the organisation, and gives us an overview of some interesting projects that are currently ongoing.

'Together we all seek answers to the deep questions that remain about the nature of matter, energy, space and time'



To start, could you please give our readers a brief introduction to Fermilab, and tell us a little bit about its history and mission?

Fermilab is a particle physics laboratory located outside Chicago, Illinois. It is one of 17 U.S. Department of Energy national laboratories, and it was founded in 1967. Fermilab builds cutting-edge particle accelerators and detectors to unravel the biggest mysteries of our universe, and to study it at the smallest and largest scales. We do this by creating particles in the laboratory using accelerators and measuring them using detectors. We also use particle detectors to search for naturally occurring particles of dark matter, and place detectors on telescopes to learn more about the mysterious phenomenon of dark energy. We build and operate world-leading facilities for the use of scientists from around the world.

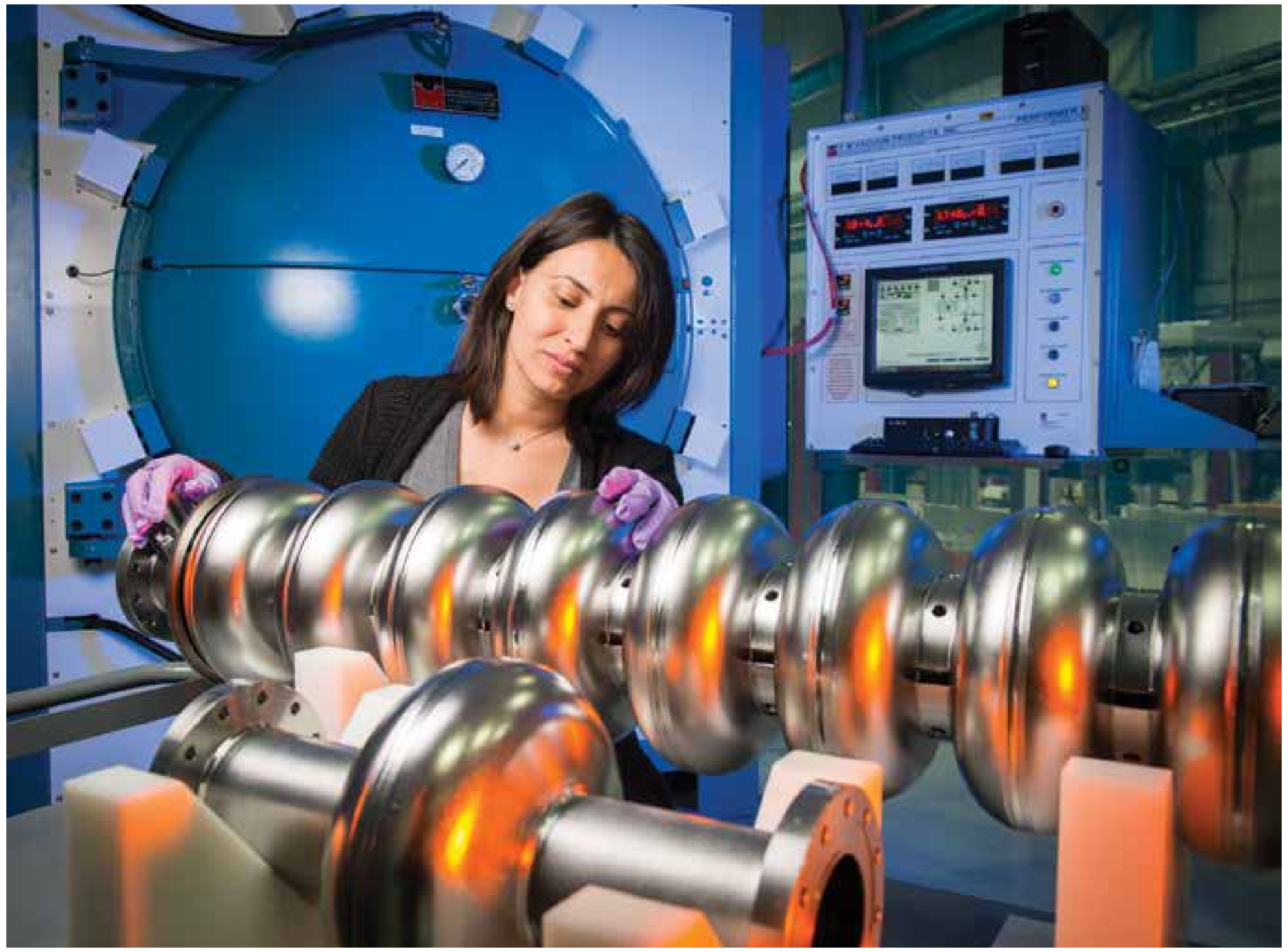
How many different countries are involved in the research conducted at Fermilab, and who are your biggest collaborators?

Fermilab works with 44 different countries, and roughly 3,500 scientists from around the world collaborate with us on our experiments. Fermilab collaborates closely with the CERN particle physics laboratory in Europe, other laboratories in Europe, North America and Asia, and scientists and students from universities around the world.

Can you tell us a little bit about the neutrino experiments that are currently ongoing at Fermilab?

Neutrinos are nearly massless fundamental particles that interact so rarely with other matter that trillions of them pass through our bodies each second without leaving a trace. They are the most abundant matter particles in the universe, but we know very little about them. For example, we know that there are at least three different types of neutrinos. But we don't know their masses – or even which one is the lightest and which is the heaviest – we don't know if there are more than three, we don't know if neutrinos and antineutrinos behave differently, and we don't know whether the neutrino is its own antiparticle. There are also theories that say that neutrinos played a big role in the evolution of the universe, but we can't say yet whether those theories are true.

All of these questions are very tantalizing to physicists, and today the study of neutrinos is a very competitive field of physics. There are experiments to study neutrinos in North America, Europe, Asia and Antarctica. At Fermilab, we currently operate neutrino experiments on our site and in northern Minnesota. We have plans to create a suite of three new on-site neutrino experiments, which will search for signs of a long-theorized fourth type of neutrino, and we are steadily working toward building our new flagship, the Deep Underground Neutrino Experiment, which will be the largest long-distance neutrino experiment ever constructed. We will send a beam of neutrinos 1,300 kilometers through the earth to South Dakota to study neutrino oscillations.



Additionally, our readers would love to hear about Fermilab's dark energy and dark matter research, please highlight one or two key projects that are currently underway.

The main project Fermilab is involved with in that realm is called the Dark Energy Survey. Scientists built and tested one of the world's most powerful digital cameras at Fermilab and then mounted it on a telescope in Chile, and they are spending five years taking extraordinarily detailed snapshots of the cosmos. They will use this data to study dark energy's effect on the universe over time, as it has pushed galaxies and cosmic structures away from one another. The Dark Energy Survey is also using this data to make a map of dark matter concentrations in the survey area.

We are also involved in several next-generation experiments to search for particles of dark matter, including a next-generation experiment being built in the SNOLAB underground research facility in Canada.

In 2008, scientists at Fermilab discovered a new sub-atomic particle – the bottom Omega baryon. Please could you explain to us why this finding was so significant?

Every newly discovered particle is an important piece of information leading to a clearer picture of how the universe works. The bottom Omega baryon is a composite particle, containing different combinations of quarks. By discovering different types of composite particles and measuring their properties, we learn more about how fundamental particles come together to make up everything we see (and don't see) in the universe. Fermilab has also been the place that three truly fundamental particles were first observed, including the top quark, the bottom quark and the tau neutrino.

How was Fermilab involved in the discovery of the Higgs boson in 2012?

Fermilab is the US hub for the Compact Muon Solenoid (CMS) experiment, one of the two that discovered the Higgs. Fermilab scientists made vital contributions to the construction of the Large Hadron Collider, including the superconducting magnets that focus particle beams into collision. Fermilab also make major contributions to the construction of the CMS detector, and roughly 100 Fermilab employees work on the CMS experiment itself. Fermilab also serves more than 500 US scientists who work on the CMS experiment through its remote operations centre that lets US scientists and students monitor scientific data as it is collected in real-time thousands of miles away in Europe, and through its computing centre that is one of the top in the world for LHC data, processing and analysing millions of collisions a second in real time. Fermilab scientists, technology and expertise were a major part of making the Higgs discovery happen.

On a different note, is it true that the Fermilab site is open to members of the public? Please tell us a little bit about Fermilab's position on public engagement.

Fermilab is strongly committed to public engagement. Much of our 6,800-acre site is open to the public every day. We offer free public tours once a week, and a free 'Ask a Scientist' event on the first Sunday of each month. We offer public events regularly, from our well-attended Family Open House to our public arts and lecture series to our work with every school in our local area. Fermilab also has a Community Advisory Board made up of local citizens who offer their perspectives on our interactions with the community.

Also, could you please tell our readers about Fermilab's efforts in wildlife conservation?

Fermilab's site contains about 1,000 acres of restored tall grass prairie and a further 1,000 acres of woodland and wetland, and it is home to many different varieties of wildlife. We employ an ecologist and work with a non-profit group called Fermilab Natural Areas to keep those areas diversified and beautiful. We also have a (fenced-in) herd of bison on site, which is quite an attraction for the local community.

Finally, can you please share your thoughts on the future of fundamental physics research, and the ongoing role of Fermilab in that future?

For nearly 50 years, Fermilab has been a world leader in discovery science, seeking out answers to the fundamental questions about our universe. Interest in our particular type of science (particle physics) is very high right now, with the discovery of the Higgs boson and last year's Nobel Prize in physics being awarded for neutrino research. The future of physics is very bright, and it is also highly international – all of the world's major particle physics projects are being built through international collaboration and cooperation. As we work toward the future flagship Deep Underground Neutrino Experiment we are becoming a truly international laboratory. More than 25 countries are already on board with DUNE and we are actively seeking to engage more partners. Together we will all seek answers to the deep questions that remain about the nature of matter, energy, space and time.

All photos courtesy of Fermilab

Fermilab

www.fnal.gov

THE EUROPEAN SOUTHERN OBSERVATORY


Credit: ESO/H.H. Heyer

The European Southern Observatory (ESO), is an intergovernmental organisation that facilitates astronomy and astrophysics research. Since its creation in 1962, ESO has provided scientists with the world's most powerful ground-based telescopes in its host state of Chile, where they can avail of exceptional observing conditions. Richard Hook at ESO tells us all about the organisation, some ground-breaking discoveries made, and what the future holds for astronomy and astrophysics research.


Credit: ESO

'One of the biggest challenges will be the search for Earth-like planets around other stars and possible detection of evidence of life elsewhere in the Universe'

Firstly, could you please briefly introduce ESO, and tell us a little about its history, focus and scope?

The European Southern Observatory is the foremost intergovernmental astronomy organisation in Europe and the world's most productive astronomical observatory. Our main mission, laid down in the 1962 Convention, is to provide state-of-the-art research facilities to astronomers and astrophysicists, allowing them to conduct front-line science in the best conditions. The organisation is supported by Austria, Belgium, Brazil, the Czech Republic, Denmark, Finland, France, Germany, Italy, the Netherlands, Poland, Portugal, Spain, Sweden, Switzerland and the United Kingdom, along with the host state of Chile. Several other countries have expressed an interest in membership.

Over the nearly 54 years of its existence, ESO has taken European ground-based astronomy from being a relatively minor player in a world dominated at that time by the US to a world-leading position. It has brought the European astronomical community together so that it can tackle projects that are far beyond the reach of single countries.

ESO operates three unique observing sites in Chile: Paranal, La Silla and Chajnantor and has its Headquarters in Garching bei Munchen, Germany. Its observatories are located in Chile because of the exceptional observing conditions to be found in the north of the country, which are unequalled anywhere else in the southern hemisphere. By building and operating a suite of the world's most powerful ground-based astronomical telescopes enabling important scientific discoveries, ESO offers numerous possibilities for technology spin-off and transfer, together with high technology contract opportunities and is a dramatic showcase for European industry.


Credit: ESO

Who are your main collaborators, and how does ESO promote co-operation between researchers across different disciplines and from different institutions?

We work closely with both academic communities and industry in the ESO's Member States. Our vision also entails expanding our scientific reach to additional disciplines such as solar physics, cosmic ray physics and ultra-high energy astronomy, and to contribute to fundamental physics.

Training is an important part of ESO's mission. We have been running a successful Fellowship and Studentship Programme for the last three decades that is exemplary in Europe. We also provide strong support for young scientists to perform research in astronomy, to help them become leading scientists for the benefit of their home countries and beyond. In addition, we have a vigorous programme of international conferences with themes in front-line astronomical science and technology and provide logistic support for the international journal Astronomy & Astrophysics.

Where does ESO receive its funding from, and what counties are involved?

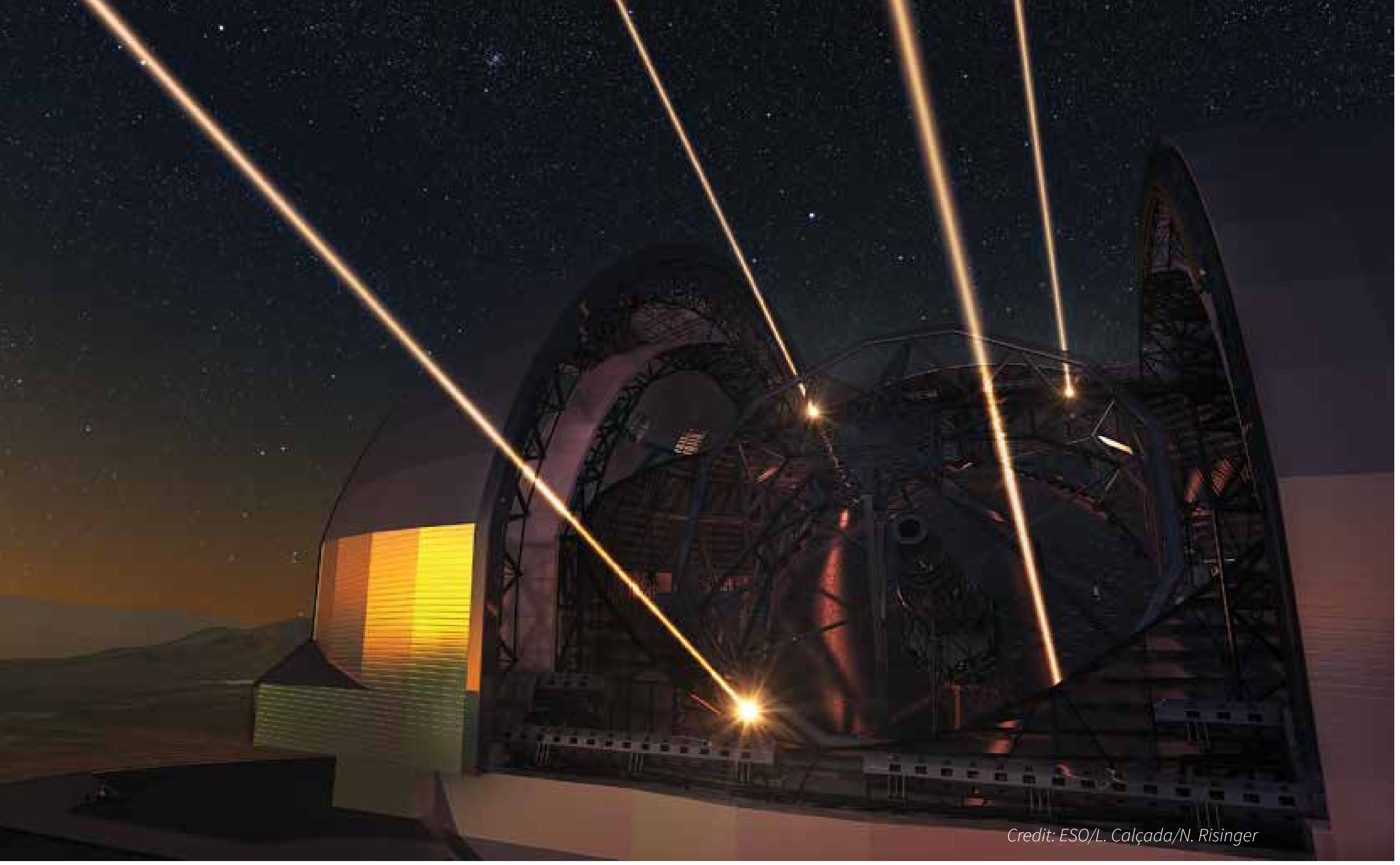
ESO is primarily funded by contributions from its Member States. The total annual Member State contributions to ESO are approximately 150 million euros, or about 0.20 euros per person in Europe per year.

Please highlight a few exciting projects that are currently ongoing at ESO.

This is an exciting time for ESO and the future is looking bright.

ESO's flagship observatory at Paranal in northern Chile is the home of the Very Large Telescope, the VLT. The VLT is the most productive individual ground-based facility and leads to the publication of (on average) more than one peer-reviewed scientific paper per day.

We are also a partner in ALMA – a



Credit: ESO/L. Calçada/N. Risinger

revolutionary astronomical telescope comprising an array of 66 giant 12-metre and 7-metre diameter antennas observing at millimetre and submillimetre wavelengths (from radio waves to far-infrared radiation). ALMA is the most powerful telescope for observing the cool Universe – molecular gas and dust as well as the distant Universe. It is sited on the Chajnantor Plateau, at 5000 metres altitude in the Chilean Andes. ALMA started its scientific observations in 2011 and was inaugurated in 2013. It is now fully operational and delivering transformation science in many areas.

ESO is now constructing the European Extremely Large Telescope, the E-ELT, which will be largest optical/near-infrared telescope in the world – the world's biggest eye on the sky. The E-ELT will have a main mirror 39 metres in diameter. The green light for the construction of this vast telescope was given in late 2014, and the construction is expected to take about ten years. The E-ELT is being built on Cerro Armazones, just 20 kilometres from Paranal.

Describe one or two of the biggest breakthroughs that the ESO has been involved with over the past few years.

ESO facilities have been used for many breakthroughs. Among the most significant are its involvement in the discovery of the accelerating expansion of the Universe, the study of the environment of the four-million solar mass black hole at the centre of the Milky Way and the first image of a planet outside the Solar System.

What are the greatest challenges facing astronomy and astrophysics research today?

This is an exciting time for astronomy, with many new facilities becoming available and new research areas opening up. For ESO, the next decade will be dominated by the technical challenges associated with building the E-ELT, whilst continuing to support and improve its other, very productive, existing facilities. No-one has built such a large telescope before.

Scientifically, one of the biggest challenges will be the search for Earth-like planets around other stars and possible detection of evidence of life elsewhere in the Universe. New facilities such as the E-ELT are bringing this extraordinary possibility tantalisingly close. Looking further afield, the challenge of trying to understand the nature of mysterious

Credit: ESO

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www.eso.org/

Credit: ESO/B. Tafreshi

dark matter and dark energy, which make up the bulk of the Universe, will keep astronomers busy for a long time!

Considering the great variety of astronomy and astrophysics research that is undertaken worldwide, how does ESO ensure that resources are best allocated?

Astronomers worldwide compete for time on ESO facilities, and requests for time greatly exceed the time available. Proposals are assessed by groups of experts – this ensures that ESO facilities are always devoted to addressing the most relevant and effective scientific projects. Our activities are continuously reviewed by experts and members of the astronomical community.

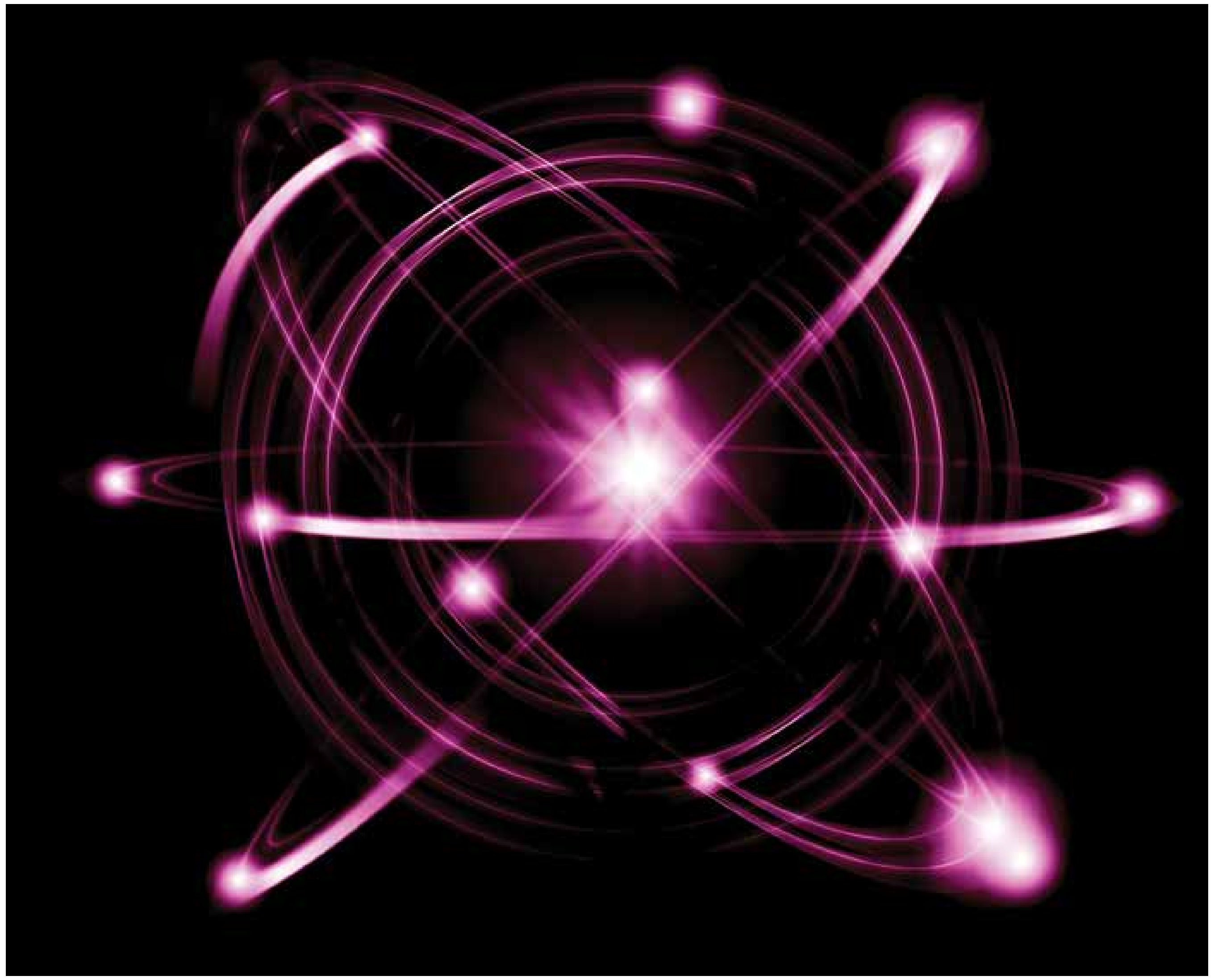
Please tell us a little bit about the ESO's position on public engagement and knowledge dissemination?

We have a very active outreach department that produces about 50 press releases per year along with many other products, including spectacular images, video material (including very popular podcasts) and printed material. The outreach group also supports many media and VIP visits to the observatory sites in Chile.

We are also in the process of constructing a state-of-the-art planetarium and visitor centre at ESO Headquarters in Garching – the ESO Supernova Planetarium & Visitor Centre. The ESO Supernova is made possible by cooperation between ESO and the Heidelberg Institute for Theoretical Studies (HITS). The building is a donation from the Klaus Tschira Stiftung and ESO will run the facility. The ESO Supernova will open to the public in late 2017.

Finally, can you please share your thoughts on the future of astronomy and astrophysics, and the ongoing role of ESO in that future?

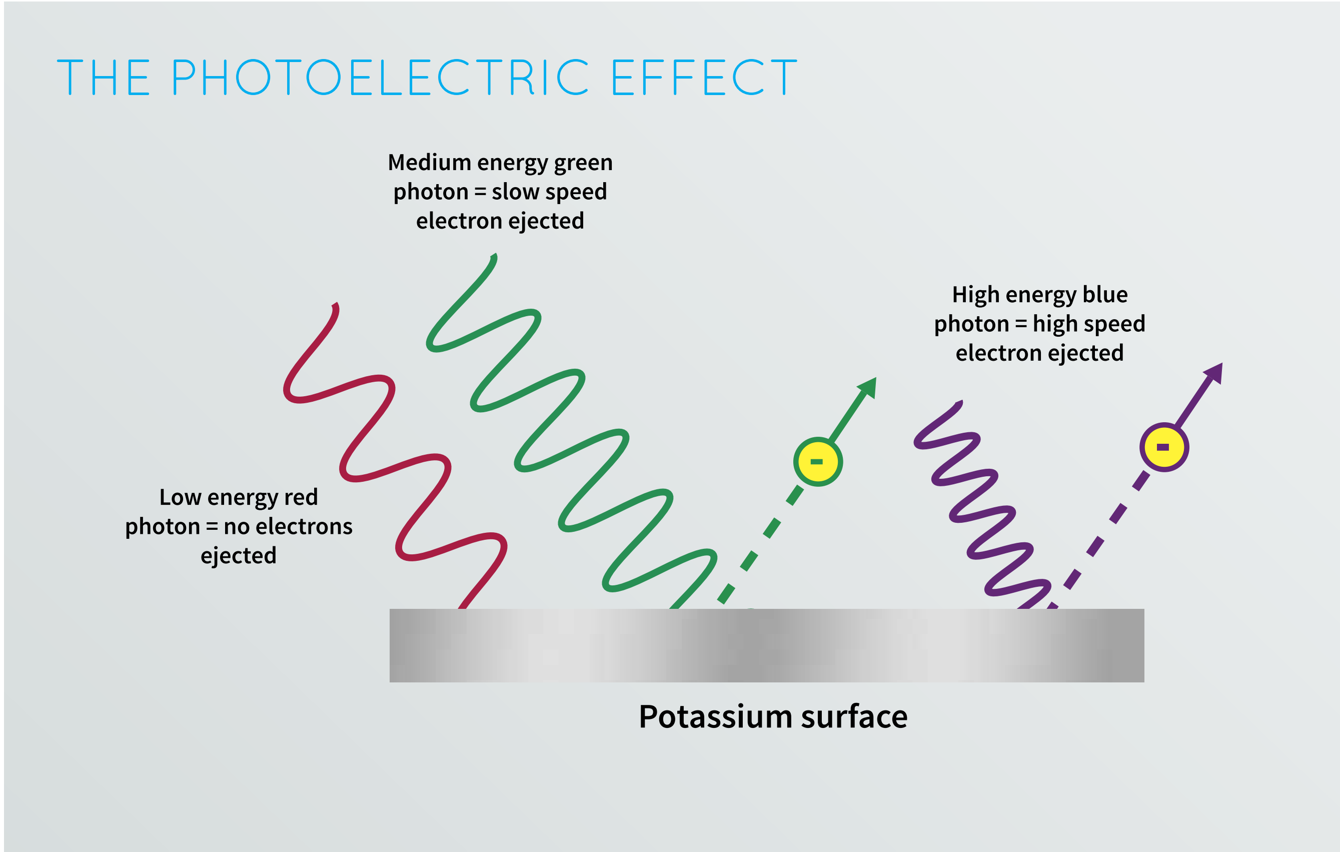
As mentioned, this is an exciting time for astronomy, and new facilities such as the E-ELT will both allow astronomers to address many of the crucial questions of today and also to make unexpected discoveries that will drive the subject forward into areas not currently imagined. ESO, as the pre-eminent ground-based observatory, will have a huge role to play in this process.



QUANTUM QUESTIONS

The bewildering field of quantum mechanics first emerged at the dawn of the 20th century, and its origins can be credited primarily to Max Planck. His theory, which revolutionised our understanding of atomic and subatomic processes, all started with his investigations into the problems associated with black-body radiation. Up until then, the theory of classical electromagnetism, which assumed light to be a wave, failed to explain how the frequency and intensity of light emitted from a black-body was dependent upon the temperature of the black-body. Take a fireplace poker for example (an approximate black-body radiator) – at room temperature it emits low energy infrared radiation, but after heating it in the fire for a period of time, it can glow in the red, yellow or even blue regions of the visible spectrum, depending on its temperature. Planck's explanation for this, which he presented to him peers in 1900, relied on the assumption that electromagnetic energy could only be emitted in quantised form. Specifically, energy can only exist as a multiple of an elementary unit, or quantum, given by his equation $E = h\nu$, where ν is the frequency of the light emitted and h is the proportionality constant devised by Planck, aptly named the Planck constant.

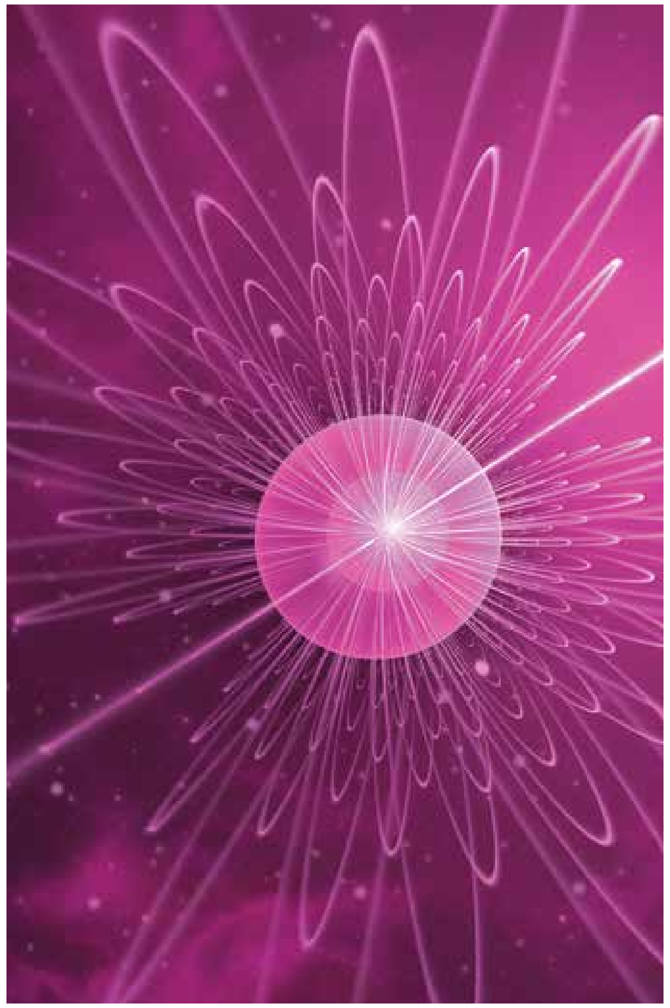
However, Planck had very little faith in his hypothesis, which he considered to be a mathematical trick employed simply to make the figures fit. Then, just five years later, Albert Einstein used the quantum hypothesis to explain a phenomenon known as the photoelectric effect, in which shining a light on certain materials can cause electrons to become ejected from their surfaces. Einstein explained this observation by suggesting that a beam of light is actually composed of individual packets of energy, and their energy is proportional to the frequency of the light. These discrete packets or quanta of light are now known as photons. Photons carrying energy above a threshold for a certain photoelectric material can knock electrons from



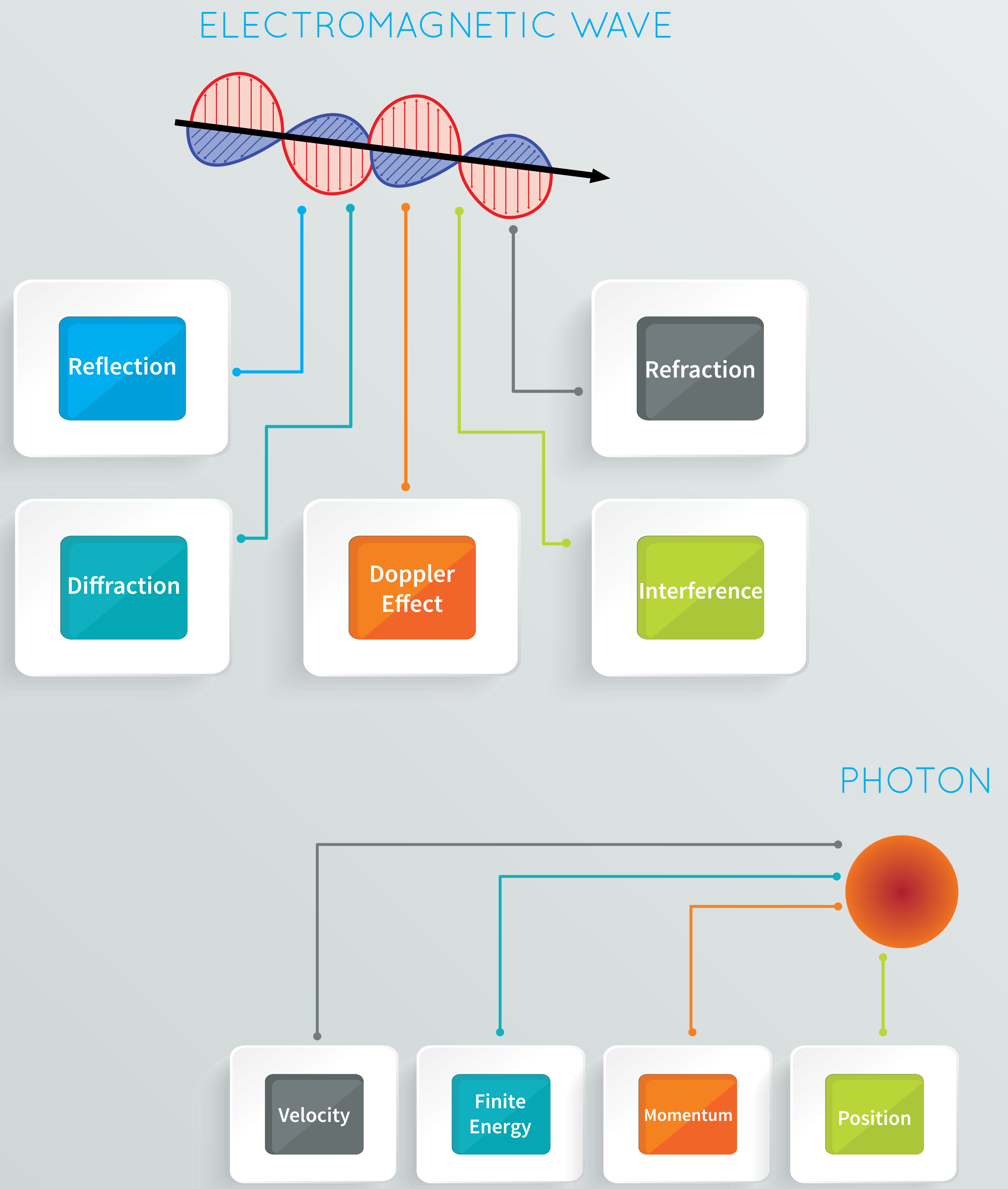
their orbits, while photons of lower energy are unable to do so, regardless of the intensity of the light beam.

However, although it was determined that photons have particle-like properties like momentum and position, they still exhibit wave-like characteristics such as frequency, refraction, interference and polarisation. Planck and Einstein's ground breaking work lay the foundations for the concept that subatomic particles and electromagnetic waves are neither particles nor waves, but have properties of both. Thus, the concept of wave–particle duality was born.

Today, quantum mechanics is the mathematical foundation of many fields of physics and chemistry, and many applications rely on our understanding of quantum phenomena, including superconducting magnets, lasers, LEDs, transistors, semiconductors and many imaging techniques such as MRI. In this section we showcase the work of Professor Hirofumi Sakai, who focuses on controlling quantum phenomena in molecules. By carefully manipulating the orientation of molecules using lasers and electric fields, Professor Sakai and his team are increasing our fundamental knowledge of how quantum processes operate on a molecular level. Next, we introduce Professor Takashi Sato, who harnesses a property exhibited by diode lasers called quantum noise, to develop high speed number generators. His fascinating research may lead to the development of better encryption systems for data security. Finally, we introduce Dr Ryoma Hayakawa, who applies quantum technology to the development of faster computing devices. His fascinating research involves employing single molecules as electronic components in transistors and memory devices, making it possible to control circuits at the level of individual electrons. These innovations could lead to revolutionary new approaches to computing.



WAVE-PARTICLE DUALITY OF LIGHT



Manipulation of Molecular Quantum States

Hirofumi Sakai is associate professor and group leader at the Department of Physics, Graduate School of Science, the University of Tokyo, where he is an expert in high-intensity laser physics, and molecular optics.

How did your research begin in molecular alignment and orientation?

The starting point came with the success of the deflection of neutral molecules using the non-resonant dipole force. Deflection of neutral molecules means controlling the centre-of-mass motion of neutral molecules. This experiment was done in the National Research Council (NRC) of Canada, where I was working as a visiting researcher with Dr. Henrik Stapelfeldt and Dr. Paul B. Corkum.

Through experiments using the non-resonant induced dipole force, I came to know that the non-resonant induced dipole interaction can be used to manipulate neutral molecules, which has many applications and led to rapid progress in molecular alignment and orientation.

After realising that the non-resonant induced dipole interaction can be used to deflect molecules, I was eager to demonstrate the molecular alignment for the first time. A two-dimensional ion imaging apparatus is very useful in evaluating the degrees of alignment based on the angular distributions of the fragment ions, produced from multiply-ionised aligned molecules in a process called Coulomb explosion. At that time, Stapelfeldt, who was one of my collaborators in NRC, started work at Aarhus University, Denmark, and developed a velocity-map ion imaging spectrometer. I worked as a visiting researcher at Aarhus and we succeeded in demonstrating molecular alignment. After leaving, my colleagues there succeeded in demonstrating three-dimensional molecular alignment with an intense non-resonant elliptically polarised laser pulse.

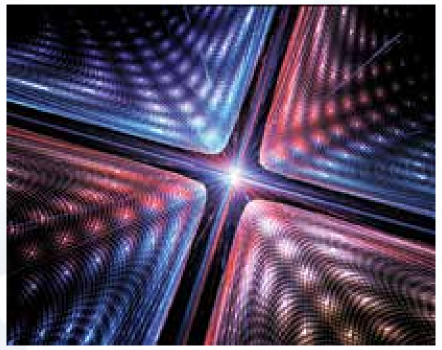
Can you tell us about how your career has progressed since then and what your new results are?

In October 1999 I moved to the University of Tokyo to develop various molecular orientation techniques. Using a theoretical proposal by Friedrich and Herschbach, our group demonstrated one and three-dimensional orientation of ordinary molecules. This was done with linearly and elliptically polarised laser fields, respectively, in a weak electrostatic field (the combined-field approach) in the adiabatic regime. Based on these results, our group proposed and demonstrated laser-field-free molecular orientation with an intense non-resonant laser field, which has a slow turn-on and a rapid turn-off in a weak electrostatic field.

Then in order to increase the degrees of orientation, we used a sample of iodobenzene molecules in their lower rotational states, which were selected by our homebuilt molecular deflector. By applying the plasma shutter technique, we achieved laser-field-free orientation of state-selected asymmetric top molecules. More recently, we have achieved laser-field-free three-dimensional orientation of state-selected asymmetric top (3,4-dibromothiophene) molecules, with an elliptically polarised laser field. This accomplishment marks the acme of molecular orientation techniques based on the combined-field approach because all the desired requirements, such as laser-field-free condition, three-dimensional control and higher degrees of orientation, were successfully achieved. From here we want to develop a novel method to efficiently orient gaseous molecules at higher densities, above 10^{17} cm^{-3}, and higher rotational temperatures, above 10 Kelvin.

Why were state-selected asymmetric top iodobenzene molecules used in your experiments?

In general, molecular orientation is much more difficult than molecular alignment. The reason for the additional difficulty is that molecules in their initial rotational states are oriented in different directions. In order to overcome this to increase the degree of orientation, it is useful to select molecules in lower rotational states using the molecular deflector we developed. We used state-selected asymmetric top iodobenzene molecules as a sample. The reason for using asymmetric top molecules as a sample is that an asymmetric top molecule is the most general



molecule in the classification based on the magnitude of the moment of inertia.

What other research avenues are you exploring in molecular alignment and orientation?

As an alternative molecular orientation technique, our group has proposed and demonstrated all-optical molecular orientation with an intense non-resonant two colour laser field in the adiabatic regime. The technique relies on the combined effect of the anisotropic hyper-polarisability interaction as well as the anisotropic polarisability interaction. By employing state-selected molecules as a sample and by operating the plasma shutter at the peak of the two-colour pump pulse, completely field-free molecular orientation with higher degrees of orientation will be achieved just after the rapid turn-off of the pump pulse.

What is perhaps the most interesting immediate application of your research?

It is said that “seeing is believing” and many researchers are now interested in making “molecular movies” with X-ray free electron laser radiation to understand ultrafast structural dynamics in laser-molecule interactions. Molecular movies are made from many frame-by-frame X-ray photoelectron diffraction patterns from a sample of aligned/oriented molecules using X-ray free-electron laser pulses.

Rapid Laser Switch-off Leaves Molecules well Orientated

Hirofumi Sakai of the University of Tokyo covers new ground in molecular orientation using combined field techniques, pulse shaping and in-house equipment that he and his group have pioneered.

MOLECULAR ORIENTATION

Hirofumi Sakai is Associate Professor at the Department of Physics, Graduate School of Science, the University of Tokyo. Sakai's group undertakes fundamental research into a wide range of atomic and molecular physics, and quantum optics, with a focus on controlling quantum processes in atoms and molecules. In particular, they research high-intensity laser physics by studying nonlinear and ultrafast phenomena, laser control of ultrafast dynamics using shaped pulses, and imaging the structure and dynamics of molecules. In addition, they aim to "film" so-called molecular movies by means of X-ray photo-electron diffraction. The subject of their most recent research is the development of a laser-field-free technique for the alignment and orientation of asymmetric top iodobenzene molecules. Their approach to state-selected asymmetric top molecules has wide implications, as this field produces the most modern and important applications stemming from quantum physics.

The field of molecular alignment and orientation has been advancing in recent years, with established and innovative techniques that are reaching greater efficiencies and finding novel applications. The goal of molecular alignment and orientation is to manipulate an ensemble of molecules with the use of lasers and electric fields, and to rotate them so that they are lined up along the same axis. Molecular alignment is the condition where the molecules are aligned along the same axis, so some fraction of the molecules will be facing in the opposite direction. Greater control is exhibited in molecular orientation – as opposed to molecular alignment – because the molecules, as well as being aligned, will also be pointing in the same direction.

It all started for Sakai when he was working as a visiting researcher at the National Research Council, Canada, with Dr. Stapelfeldt and Dr. Corkum, on non-resonant manipulation of neutral molecules. It was there he realised that an induced dipole interaction can be used to deflect molecules, and he has since worked in this area with great interest.

NEW RESULTS

In Sakai's recent work he experimentally demonstrated the orientation of iodobenzene molecules, which have the chemical formula C_6H_5I, and possess a benzene ring structure substituted with a single, large iodine atom. The ensemble of iodobenzene molecules was originally primed for orientation by being prepared in particular rotational states by a molecular deflector that was built by Sakai and his group, which filtered out lower-lying rotational states that are easier to orientate. Lower-lying rotational states of molecules have lower rotational energies and are near the ground state.

According to Sakai, one of the reasons for choosing iodobenzene is that this molecule has "a larger anisotropic polarisability, which leads to a larger induced dipole moment, making it relatively easy to handle". In other words, the molecule is polarised, having one electrically positive end and one negative end. The more pronounced the polarisation is, the easier it is for an electric field to get a better grip and rotate the molecule into the desired orientation.

Molecular orientation is induced by an intense nanosecond laser field in a weak electrostatic filed, which is called a combined field approach. Rapidly switching off the laser field leaves the molecules in a laser-field-free state of orientation. The rapid switch-off is done by customising the shape of the laser profile using a plasma shutter technique. Sakai explains that this works with two lasers used together: "a femtosecond Ti:sapphire pulse and a nanosecond Nd:YAG pulse are collinearly focused onto an ethylene glycol jet sheet with a thickness of 50 micrometers. The intense Ti:sapphire pulse triggers the plasma formation at the peak of the YAG pulse. After that, the YAG pulse cannot pass through the plasma so it gets rapidly switched-off, in a falling time of approximately 150 femtoseconds". In other words, as the two parallel lasers are focused onto the jet sheet, the Ti:sapphire rapidly produces a plasma from the sheet that is opaque to the Nd:YAG laser, forcing it to rapidly switch-off in 150 femtoseconds, or 150×10^{-15} seconds, leaving the iodobenzene molecules in a laser-field-free state.

Once the molecules are in a laser-field-free state, they are still being oriented for a while in a dephasing time of 5–10 picoseconds, or $5–10 \times 10^{-12}$ seconds. Although this is an incredibly short period of time, it is actually a long time for molecules to be orientated under these conditions, and almost one hundred times longer than it took to rapidly turn the laser off.

The degree of molecular orientation of the whole ensemble, and the dephasing time taken by the molecules to jostle out of orientation, were measured in an interesting way using Coulomb explosion of the molecules which was detected by a two-dimensional ion imaging detector. This was done with an intense femtosecond probe pulse that was fired into the orientated ensemble to ionise the molecules in a way that caused the component iodine atoms to undergo an explosive electric repulsion from the molecular ions. The positive iodine atoms were accelerated towards a sensitive, two-dimensional detector and the image on the detector was recorded by a CCD camera. The detection position of the iodine ions was used to build up a "molecular map" that shows how the molecules are aligned or oriented by where the ions impact and cluster on the detector. The map will correspond directly to where the iodine atoms are inside the iodobenzene molecules. For a well-orientated ensemble, iodine atoms will be in the same relative positions in the sample of orientated iodobenzene molecules. The iodine atoms can be clearly distinguished from other molecular fragments from the Coulomb explosion, by their longer time of flight due to their comparatively large mass. Using experimental data, Sakai and his team calculated a maximum value of 0.68 out of 1 for the ensemble orientation which shows high orientation.

This is the state of the art in the combined field approach to molecular alignment and orientation.

ORIENTATION TOWARDS THE FUTURE

Altogether, by judiciously choosing the right parameters, such as the pulse shape and intensity of the laser-field, the strength of the electrostatic field, the initial rotational states prepared by the homebuilt deflector, and a number of other important parameters, Sakai and his team will finely tune their apparatus to prepare a better orientated ensemble of iodobenzene molecules.

More recently, and using similar techniques to those that were used here, Sakai and his team have demonstrated three-dimensional orientation of state-selected asymmetric top molecules, this time using 3,4-dibromothiophene molecules, in a laser-field-free state with an elliptically polarised laser and a weak electrostatic field. This is the state of the art in the combined field approach to molecular alignment and orientation.

These results will be of great interest to those working in chemical stereodynamics, where chemical reaction rates that depend on the spatial orientation of molecules are studied. There are many more important areas of research that can benefit from these techniques, such as high-order harmonic generation, non-sequential double ionisation, hot above-threshold ionisation, and two-electron excitation. An interesting and recently considered application is making "molecular movies" using X-ray photo-electron diffraction, for the purposes of displaying molecular dynamics in real-time that can be watched just like a movie. Being able to watch molecular movies may give confirmation and new insights into molecular dynamics. As Sakai has carried out research in these areas, he and his group are well placed to make breakthrough contributions.

Researcher Profile

Dr. Hirofumi Sakai
Department of Physics, Graduate School of Science
The University of Tokyo, Japan

Dr. Hirofumi Sakai is Associate Professor at the University of Tokyo, Japan, and specialises in experimental studies of quantum optics and atomic/molecular physics, the papers of his group in Tokyo gathering worldwide attention and about 1300 times of citations. He received his Ph.D. in science from the University of Tokyo in 1994, after which he remained to continue his research career in quantum optics and atomic and molecular physics. His research interests include the ultrafast-laser control of molecular quantum processes, nonlinear high-intensity laser physics and ultrafast atomic and molecular phenomena.

CONTACT
E: hsakai@phys.s.u-tokyo.ac.jp
T: +81 3 5841 8394
W: http://www.s.u-tokyo.ac.jp/en/lp/sakai_hirofumi/
W: http://www.amo-phys-s-u-tokyo.jp/en/

KEY COLLABORATORS
Prof. Paul B. Corkum, University of Ottawa and National Research Council of Canada, Canada
Prof. Henrik Stapelfeldt, Aarhus University, Denmark
Prof. Eric Constant, Université de Bordeaux, France
Prof. Jakob Juul Larsen, Aarhus University, Denmark
Dr. C. P. Safvan, Inter University Accelerator Centre, India
Dr. Shinichirou Minemoto, The University of Tokyo
Acknowledgements to all the graduate students for molecular orientation and other related studies at the University of Tokyo

FUNDING
Japan Society for the Promotion of Science (JSPS)
Ministry of Education, Culture, Sports, Science, and Technology (MEXT)

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Taking full advantage of current technology

Diode lasers are one of the most important objects modern technology has to offer. Dr. Takashi Sato of Niigata University, in Japan, studies and creates devices based on diode lasers, thinking of ways to improve what we can do with this technology. The use of diode lasers to design better physical random number generators and optical communications systems are examples of his work.

What is your research background? How did this lead you to design diode laser devices and study their properties?

In 1960, I was a first-year elementary school student when I heard the news about the "best invention of the twentieth century" – the LASER (Light Amplification by Stimulated Emission of Radiation). That was when I decided I wanted to do some research on it. That was the beginning of it all.

Double optical feedback to a Vertical Cavity Surface Emitting Laser (VCSEL) – a type of laser with beam emission perpendicular to its top surface - seems like a very good prospect for future applications in optical communication systems. How did you come up with the idea for the project? Does this device plays any special role in current research?

As I was looking for ways to control diode lasers' oscillation frequencies without any active devices in its system, I found a paper that described a system using a double- instead of a single-optical feedback. I was also interested in VCSELs and finding ways to control their oscillation frequencies. The difficulties of introducing the VCSEL to the double optical feedback system seems to lay in VCSEL's highly reflective mirrors. And, even though the reflectivity of a Fabry-Perot etalon (a type of diode laser) is also very high, we can observe the transmitted light through it at its resonant mode. Therefore, we tried to introduce a VCSEL into our double optical feedback system.

If this device (or a modification) can be applied as a high-speed optical communication system light source, what do you think are the greatest implications of that for modern science and technology?

Both the VCSEL and its two-dimensional array structure demonstrate good multiplexing characteristics; this means a lot more data could be transmitted in several communication systems. Increasing the speed we transmit data, the possibilities are endless.

Why study random number generators? There are pseudo-random number generators. Why are the physical generators so much better?

Integers created by pseudo-random number generators can be decoded, given sufficient time. We must contend with the never-ending threat from hackers equipped with state-of-the-art computers, and advanced algorithms, who do everything in their power to access critical data. Currently, the high-speed generation of physical random numbers is one of the prospective means of accomplishing this.

Which of your research projects do you expect to be the most successful? Do you plan to extend this work further? In what direction do you plan to extend it?

Diode lasers, including the VCSEL-types, are marked by unique oscillation frequency characteristics, i.e., very fast frequency noise, so we need to be able to reduce and control it. Moreover, since they are so special, why can't we take full advantage of that? In upcoming experiments, I want to use these unique characteristics for fast physical random number generation, in a new type of rangefinder, and a light source that requires very wide frequency noise.

Making the best invention of the twentieth century better

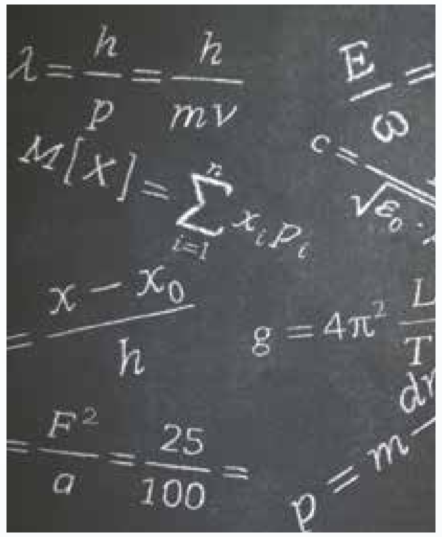
Dr. Takashi Sato proposes several new applications and improvements to a very common device – the diode laser. The diode lasers are currently present in almost all things having to do with modern technology. From your Blu-ray player to fiber optic communications and laser surgeries, they are actually found in too many uses to list all of them.

SEVERAL RESEARCH SUBJECTS ON DIODE LASERS

One of the main works of Dr. Sato is using optical feedback techniques to diode lasers. Optical feedback is, by some way, redirecting the diode laser's own light to itself, such that the quality of the final beam improves, in the sense that the frequency line width becomes very small in comparison to the frequency emitted. This basically occurs due to several reflections producing standing wave patterns for certain resonance frequencies. Then you can adjust your setup to select the frequencies that you want. Dr. Sato and his collaborators designed a double optical feedback system applied to a Vertical Cavity Surface Emitting Laser (VCSEL) – a type of diode laser that has several advantages in fabrication, compared to the more conventional one.

We must contend with the never-ending threat from hackers equipped with state-of-the-art computers, and advanced algorithms, who do everything in their power to access critical data.

Another interesting fact about diode lasers is that they have a significant amount of quantum noise in optical power and frequency. Dr. Sato took advantage of that and proposed a novel method of generating physical random numbers using diode lasers' frequency noise. His proposed setup is believed to achieve very high speeds for generation of random numbers. This could lead to several applications, especially



in the area of cryptography and protection of computer systems.

DOUBLE OPTICAL FEEDBACK TO A VCSEL

VCSEL have many advantages compared to the usual edge-emitting semiconductor laser. First, their total fabrication cost is reduced and have better process control. Second, they can be built in two-dimensional arrays, providing new applications for lasers. They also have a lower power consumption. Even though the first VCSELs had lower power emission, there has been some advancements in this subject. However, its oscillation frequency line width is broader than the best edge-emitting lasers. Dr. Sato proposed setup has many significant advantages, particularly in narrowing the oscillation line widths.

Usually, VCSELs systems are not much sensitive to optical feedback, which can be an advantage in some applications, but, if you want a very narrow oscillation line width, you have to use an edge-emitting laser. With the double optical feedback of Dr. Sato, the oscillation line width obtained (2 MHz) is compared to typical edge-emitting laser with optical feedback. Their main objective is having VCSELs that may be applied to wavelength-division-multiplex – a form of optical communications system that can have several signals (with different wavelengths) within a single optical fiber. Then, without laying more fiber, network systems can improve their capacity of communication. Dr. Sato approach can have a great impact in the application of VCSELs to this kind of technology, making VCSELs a great prospect for high-speed optical communications systems light source, since the system is inexpensive.

What happens in a double optical feedback system is that you have three modes occurring: the internal mode of the diode laser and two external modes, due to the cavities created by the mirrors. Then, if you adjust your setup, you can make a total oscillation mode with a much narrower line width, that is, you use the additional external mode to control the unwanted behaviors of the first external mode.

Through many tests, using an extremely precise measurement experimental setup, Dr. Sato and collaborators showed that double optical feedback to a VCSEL has several advantages such as suppressing low frequency fluctuation, stabilizing oscillation frequencies and, of course, narrowing oscillation line widths. There is some limitations of course, such as the actual size of the experimental setup. Nevertheless, Dr. Sato and his collaborators are working on the perspective that it can be miniaturized.

RANDOM NUMBER GENERATION THROUGH DIODE LASERS' QUANTUM NOISE

Obviously, pseudo-random number generators are not random at all. They rely on algorithms, using mathematical formulae to produce sequences of numbers that appear random, but they are actually predetermined. Because these generators are fast, they are considered efficient. However, as they are deterministic, a sequence of numbers can be reproduced, given enough resources to a skilled hacker, for instance. Nevertheless, physical number generators are based on actual random physical phenomena, which makes the numbers really unpredictable. Unpredictable, but slow. The generation of random numbers through physical phenomena takes longer time than the pseudo ones. Dr. Sato and collaborators designed a device that promises to change this.

Diode lasers have something that we call quantum noise. Emission of radiation fluctuates spontaneously, due to the quantum nature of lasers. This causes several fluctuations in the physical properties of the laser, which in turn makes the optical power and frequency fluctuate. Since the initial fluctuation is random, all the others are. Then, if there are ways of measuring these quantum noises, you can feed them to a computer to generate random sequences of numbers. It is important to note that these numbers will be truly random (this is quantum mechanics after all…), it is the equivalent of giving dice for the computer to roll.

Dr. Sato investigated this behavior of diode lasers and concluded that the oscillation frequency of the laser changes very fast, which could be used to build a high-speed physical random number generator. Using a frequency discriminator, transforming the frequency fluctuation to an intensity fluctuation, which is easier to measure, the output beam then goes to a device that converts the data to 8-digit binary numbers. They are currently producing random numbers in a speed of 3 Gbit/s, but they believe they can do much better than that.

Besides generating true random numbers, Dr. Sato's group even designed an optical range finder using the characteristics of the laser's frequency fluctuation. They compared the random data from two signals that traveled through different optical paths, one of them reflecting at a target. Because these signals originate from the same beam, their random fluctuations are correlated. Computing this correlation makes possible to determine the time lag between the optical paths. The system was accurate to a distance of up to 50 m, at a resolution of 0.03 m.

Although you can find other uses for random number generators, its main purpose is making better encryption systems. High-speed physical generators, such as Dr. Sato's device, are an important improvement for this. Security of data is maybe one of the most important things on this century, for several reasons. Encryption of data benefits from this kind of research, because, since the numbers generated are truly random, they are the definition of unpredictable. None of its sequence can be reproduced on purpose, only by chance.

Researcher Profile

Professor Takashi Sato
Niigata University
Institute of Science and Technology

Dr. Takashi Sato received his B.S., M.S. and Ph.D. in Electronic Engineering from Kyoto University. Dr. Sato aims to study and build devices, based on diode lasers, leading to applications in several fields, especially optical communications systems. He has done research with diode lasers in the subjects of frequency stabilization, oscillation frequency shift in magnetic fields, physical random number generators using frequency noise and optical range finders. His approach to diode lasers devices has the prospect of greatly improving optical and IT systems.

CONTACT
T: +81 25 262 6723
E: tsato@eng.niigata-u.ac.jp
W: http://researchers.adm.niigata-u.ac.jp/html/351_en.html

KEY COLLABORATORS
Prof. Masashi Ohkawa, Niigata University
Dr. Kohei Doi, University of Tokyo
Dr. Tomoyuki Uehara, National Defense Academy

FUNDING AND GRANTS
JSPS KAKENHI Grant 22560035 (2010-2012)
JSPS KAKENHI Grant 25390093 (2013-2015)

The middle way: combining molecular electronics with traditional silicon

Dr. Ryoma Hayakawa is an independent scientist at Japan's International Center for Materials Nanoarchitectonics. Here he discusses his attempts to realise the next generation of computer architectures.

What inspires you to work in materials science?

Materials are the basis of all productions and the evolution in our current science and technology has been achieved by the enormous discoveries of novel materials. The silicon industry now faces a major turning point owing to the critical limit imposed by increasing large-scale integration and growing power consumption.

The improvement in performance cannot be achieved by simple miniaturisation of transistors anymore. Therefore, exploring new materials is urgently required in current complementary metal-oxide semiconductor (CMOS) technology. Materials science and engineering is really essential to open up a new era in future CMOS architectures.

Why did you decide to combine traditional CMOS architectures with emerging molecular structures?

I have worked in the fields of both silicon and molecular electronics. Current CMOS technology faces a major turning point and development of new devices with novel principles is urgently required.

On the other hand, single molecular devices, which utilize single molecules as an electronic component in transistors and memories, are expected to be a promising candidate further in the future.

The development of molecular devices is, however, still at the basic research stage and practical applications remain a long way off. The main obstacle is the lack of effective device structures for molecular devices.

Hence, our approach of integrating attractive molecular functions into Si-based devices meets the requirements of both fields.

You describe the device you are trying to make as multifunctional. Why is that?

Improvement of transistor performances cannot be achieved only by miniaturization. Integration of new functionalities like multi-valued operation and integration of memory and photonic functions is necessary to push ahead with the improvement of device performances beyond the limitation in downscaling.

For this reason, we opted to use organic molecules as quantum dots to integrate attractive multifunction into future CMOS devices. The unique features of organic molecules including size uniformity, excellent controllability in energy levels, photonic functions and molecular spin manipulation, have the potential to integrate new functions into CMOS devices.

Manipulation of quantum transport with a few carriers contributes to a considerable reduction in power consumption and high-speed operation. The multi-valued operation, which is controllable by molecular orbitals, also allows further large-scale integration of electronic circuits. Adoption of photochromic molecules and magnetic ones could enable integration of optical memory and spin memory functions.

Do you think photonic and quantum technology is the future of computing?

Optical manipulations of devices are critical elements in future CMOS technology. In our study, we used photochromic molecules as optically controllable quantum dots in a Si-based double tunnel junction.

The advantage is that the energy levels of the molecules can be varied reversibly by light irradiation with specific wave lengths and the change in molecular structure induced by light irradiation can be maintained. In other words, the device works as a non-volatile optical memory. Such optical functions will be very favourable in the future.

In addition, the development of quantum transport devices is required in future CMOS devices because the devices allow extremely low power consumptions due to only having

to manipulate a few carriers. They also permit multi-valued operations with discrete levels in a quantum dot. Furthermore, the unique features such as superior controllability in energy levels, as well as photonic and spin functions, make it possible to integrate novel functions into current Si devices.

Japan is renowned for its expertise in electronics. Do you believe the country will maintain this leadership into the 'beyond CMOS' world?

Yes, I think that Japan has always been superior in the development of new materials. As we know, Japanese companies including Toshiba, NEC and Hitachi, took the lead in the field of semiconductors up to the 1980s in parallel to Intel. Now the former's share in semiconductors is occupied by many foreign companies such as Samsung Electronics. However, now is good timing for Japan to get back to the top of the field with "Beyond CMOS".

You have had to collaborate with researchers from other disciplines to further your studies. How did you find this and did it give you new insight into your research?

I have worked in the international center for young scientist at the National Institute for Materials Science, where many promising candidates with different research fields are gathering from all over the world. Collaborations with researchers with different research backgrounds give us new ideas and concepts and help us push ahead with the realization of our proposed devices.

Beyond Moore’s Law

As the inexorable capacity gains in traditional silicon electronics begin to falter, scientists are starting to search for new solutions to our computing needs. Dr. Ryoma Hayakawa is focusing on providing a bridge from the old world to the new.

CAPACITY CRUNCH

In 1965 Gordon Moore, co-founder of Intel, observed that the number of transistors per square inch on integrated circuits had doubled every year since the technology had been invented and he predicted this trend would continue for the foreseeable future.

He revised his prediction to a doubling every two years in 1975, but for decades his prediction has held firm. Now though, the continuing miniaturisation of traditional silicon electronics has begun to reach its limits as both power consumption and cost of production start to push back.

This has prompted researchers to start the search for the successor to the complementary metal-oxide semiconductor (CMOS) technology that powered last century’s computing revolution. Among them is Dr. Ryoma Hayakawa from the International Center for Materials Nanoarchitectonics, Tsukuba, Japan.

MOLECULAR ELECTRONICS

One promising avenue for taking electronics ‘beyond CMOS’ is single molecule devices, which utilises single molecules as electronic components in transistors and memories. They make it possible to control circuits at the level of individual electrons.

Such devices not only hold the possibility of dramatically reducing the size and increasing the speed of circuits, but they also demonstrate various quantum effects that could herald entirely new approaches to computing.

The development of such devices, however, is still very much at the level of basic science. A major obstacle to their widespread adoption is their lack of compatibility with standard CMOS technology. Solving this problem is the focus of Hayakawa’s work.

“Our approach meets the requirements of both fields – the incorporation of new functions into current transistors and large-scale integration of realistic molecular devices,” he says.

ORGANIC ELECTRONICS

Having worked in both the silicon and molecular electronics fields, he appreciates the benefits that both can provide. And so rather than attempting to build an entirely new architecture from the ground up Hayakawa has instead focused on integrating attractive molecular functions into silicon-based devices.

Alongside his collaborators he has integrated functional organic molecules into a metal-oxide semiconductor (MOS) structure, a basic component in current silicon transistors and memories.

The organic molecules are in the form of quantum dots – tiny particles that exhibit quantum physical effects. Traditionally these dots are made from inorganic molecules, but using organic molecules instead has several major advantages.

The molecules have a uniform size at the nanometre scale unlike their inorganic counterparts, which is important as non-uniform size hinders the ability of devices to operate in a stable way at room temperature. Uniform size also makes it possible to have a much higher density of dots, which boosts device capacities.

In addition, their energy levels are easily tuneable via the attachment of functional groups, such as electron-withdrawing or donating groups. Using photochromic or magnetic molecules also introduces the possibility of controlling the electrical properties of devices using light or magnetic fields.

“These unique features in organic molecules make them superior to inorganic dots” says Hayakawa. “Our proposed device, therefore has the potential to break through the limit of conventional silicon-technology and to integrate novel functionalities into conventional CMOS devices.”

QUANTUM CONTROL

So far the results have been promising. Hayakawa’s group has successfully demonstrated resonant tunnelling, which is a quantum transport, through molecular dots in a silicon-based double tunnel junction, where organic molecules are embedded in insulating layers in a MOS structure.

The group has demonstrated the effect in various molecules, but the most promising was their experiments with C60 molecules where resonant tunnelling was visualised even at 280 kelvin, which is almost room temperature.

In most cases transports are still limited to cryogenic temperature, but Hayakawa says the result prove the usefulness of organic quantum dots for controlling tunnelling current among other things.

“The proposed device can manipulate quantum transports such as resonant tunnelling and single-electron tunnelling,” says Hayakawa. “These features could lead to the realisation of extremely low power consumptions and high-speed operations.”

In addition the group has achieved two novel and attractive molecular functions unique to organic molecules in their silicon-based double tunnel junction - multilevel operation of resonant tunnelling and optical switching with photochromic molecules.

BOOSTING THE BITS

Current transistors and memories operate on a binary basis meaning only one bit of information can be manipulated at a time. Enabling multi-valued operation capable of manipulating multiple bits at a time could drastically reduce the number of components and interconnections on a chip enabling higher switching speeds and lower power consumption.

One way of achieving multi-valued operation is by controlling the energy levels of the molecules forming quantum dots. Organic molecules are particularly useful for this as the energy levels of these molecules can be varied markedly just by fluoridation, without changing the basic molecular frame.

Hayakawa’s group has fabricated a binary-molecule-based double tunnelling junction, in which both F16CuPc and CuPc molecules are incorporated together in an insulating layer. They observed multiple staircases reflecting the energy levels of the respective molecules, which indicates the potential for multilevel operation of resonant tunnelling with multiple molecules - something not possible with inorganic quantum dots.

“In inorganic quantum dots the interval in threshold voltages is decided by charging energy, which depends on the size of the quantum dots,” says Hayakawa. “In inorganic quantum dots, the change in dot size is a serious problem directly connected to the instability of devices at room temperature.”

LIGHTS CAMERA ACTION

The group has also experimented with optical control of resonant tunnelling using a derivative of diarylethene molecules to form optically controllable quantum dots. Importantly the optical control causes minimal change in the molecular geometrical structure so it should work even in a solid-state matrix. Their findings suggest the approach could allow the integration of photonic functionality into current silicon-based memory devices. Hayakawa says, “The construction of optical interconnection networks is a major topic because the complexity of interconnections in integrated circuits is a bottleneck for improving transistor performances. The delay in response with the increase of interconnections and the degradation of devices due to overheating are serious problems in current CMOS devices.”

Now Hayakawa is working on integrating these novel molecular functions into a vertical tunnel transistor with a double tunnel junction to realise a realistic molecular device. In recent preliminary work his group managed to fulfil basic transistor operations with their prototype.

“The most important thing is that our study demonstrates another direction in the strategy to develop future CMOS architectures,” says Hayakawa. “Our attempt has enormous potential for providing a breakthrough in silicon technology. But there are many obstacles to overcome in the realisation.”

RELATED MANUSCRIPTS

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Researcher Profile

Dr. Ryoma Hayakawa

International Center for Materials Nanoarchitechtonics
National Institute for Materials Science

CONTACT

E: HAYAKAWA.Ryoma@nims.go.jp
P: +81 29 860 4808
W: http://samurai.nims.go.jp/HAYAKAWA_Ryoma-e.html
W: http://www.nims.go.jp/mana/member/independent_scientist/ryoma_hayakawa.html

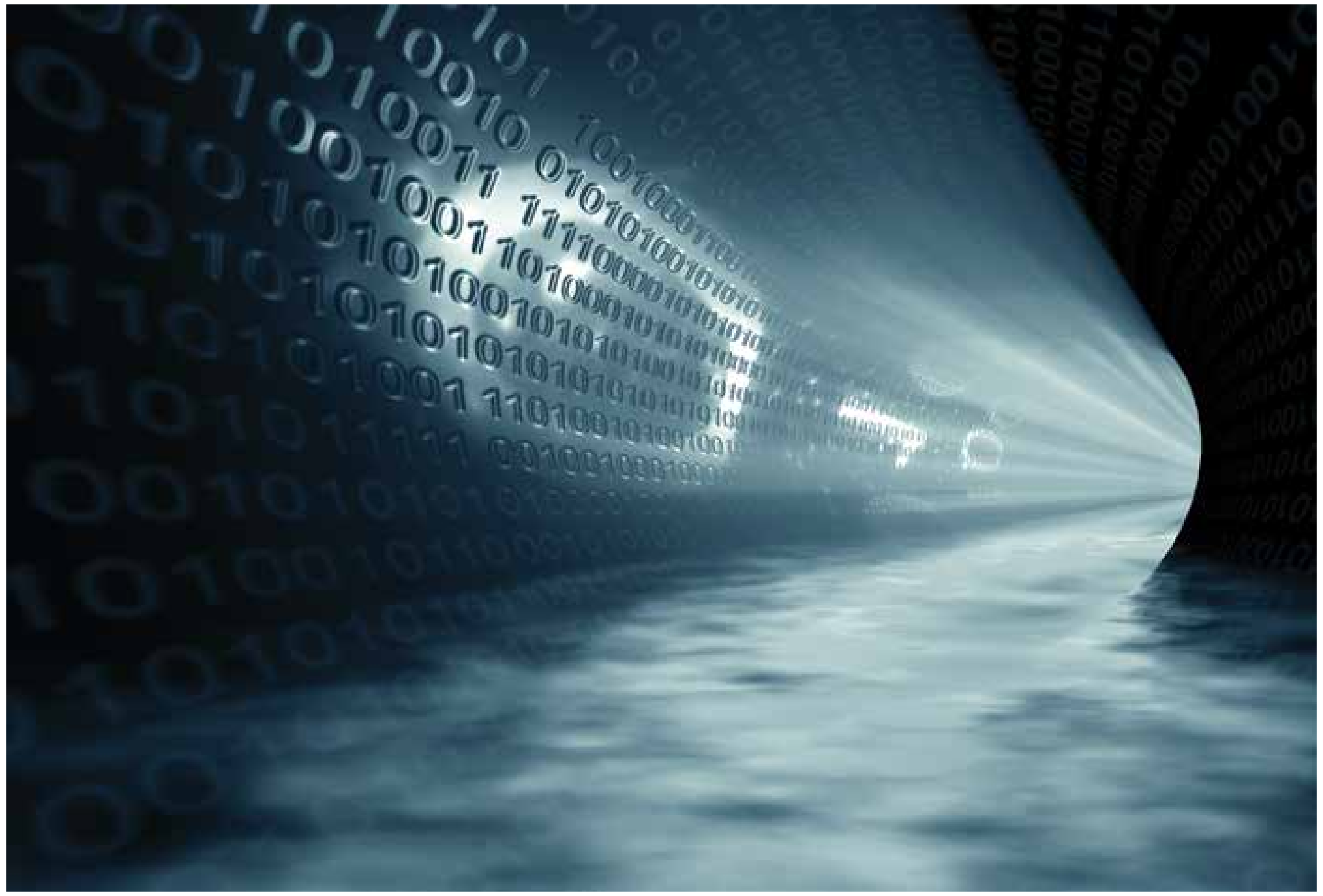
Dr. Ryoma Hayakawa is an independent scientist at the International Center for Materials Nanoarchitectonics MANA at the National Institute for Materials Science in Japan. He received his undergraduate, masters and PhD in Engineering from Osaka Prefecture University, completing his studies in 2006. His research activities are focussed on integrating molecular electronics and standard silicon electronics. He also investigates the potential of organic field-effect transistor. Alongside fellow researchers he holds patents on a method for forming oxynitride and nitride films, a type of field-effect transistor and a dual-gate organic thin film transistor.

KEY COLLABORATORS

Yutaka Wakayama, National Institute for Materials Science
Chikyow Toyohiro, National Institute for Materials Science
Kenji Matsuda, Kyoto University
Kenji Higashiguchi, Kyoto University

FUNDING

Japanese Ministry of Education, Science, Sports, and Culture,
Grants-in-Aid for Scientific Research,
The Kurata Memorial Hitachi Science and Technology Foundation,
National Institute for Materials Science



THE COMPUTING REVOLUTION

Computers define the age we inhabit. From the early pioneers, such as Alan Turing, to the latest innovators, such as Bill Gates or Steve Jobs, computers have changed the way we live and work, forever. The innovation continues apace. Computer systems available today facilitate a myriad of computational techniques with manifold applications. In this section, we demonstrate the work of three researchers who have contributed significantly to the development and application of computational systems and techniques.

The first article in this section deals with the work of Dr Edward Kansa. Dr Kansa is credited with developing a computational technique, aptly named the Kansa method, which simplifies and facilitates the computational solution of complex mathematical problems. The technique is applicable to a variety of fields, from astrophysics to quantum mechanics and biology. Next, we explore the work of Professor Hassan Noura, an expert in fault tolerant control computer systems. Fault tolerant control deals with automated fault detection, diagnosis and correction systems for automated machines, such as cars or aircraft. A major focus of Professor Noura's work is on developing systems for unmanned aerial vehicles. Finally, we introduce Dr Shoji Hamada of Kyoto University, who's research deals with computational simulation and modelling of electric fields and currents in the human body. The goal of Dr Hamada's fascinating work is to reduce or prevent harm to the human body from electric or electromagnetic fields, from devices such as defibrillators, and maximise their effectiveness.

COMPUTATIONAL METHOD CURES THE CURSE OF DIMENSIONALITY

Dr Edward Kansa, winner of a George Green medal, has worked for decades on a fuller application of smooth radial basis functions with wide applicability in engineering, computer science, and physics – the powerful Kansa method.

The Kansa method for engineers and physicists

Dr Kansa began his career by earning a PhD at the Vanderbilt University with a thesis in many-body quantum physics. Following his PhD, he worked at the United States Bureau of Mines as a research physicist. There, he used his understanding of applied mathematics and physics to model coal dust fires and explosions. Later on, his work at the Lawrence Livermore Laboratory focused on modelling natural gas explosions, the spread of pollutants in ground water, earthquakes, the safe deposition of spent nuclear reactor fuel, and the problem of tank ruptures and ammonia spills. During his career, he held teaching positions with the University of California's Department of Mechanical and Aerospace Engineering and with Embry-Riddle Aeronautical University's Department of Physical Sciences, in Oakland, California.

Dr Kansa's work faced him with some of the most computationally complex and challenging applied mathematical problems, namely dynamical systems and fluid dynamics. Apart from their countless applications in physics and engineering, fluid dynamics and dynamical systems are still open areas for research, which means they sometimes pose problems that are not readily solvable through known, closed form methods. The main difference between fluid dynamics and dynamical systems is their domains of applicability. While fluid dynamics can model the flow of water through a pipe, dynamical systems address the problem of avalanches in sand piles, or other types of complex time evolutions, for example attractor maps or the orbital motion of planets.

To illustrate properly the importance and challenges of research in fluid dynamics one has to know that this is one of the Millennium Prize problems. Only 6 still open problems in pure mathematics or mathematical physics are considered attention worthy enough to be part of this prize. The mathematician solving any of these open problems, among which are the Navier-Stokes equations governing fluid dynamics, will receive a noteworthy cash reward and will most likely remain in the history books.

However, solving the open problems in fluid dynamics and dynamical systems does not guarantee that these problems are computationally easier to approach. In fact, they would still be extremely computationally intensive. And this is where Dr Kansa's work comes in.

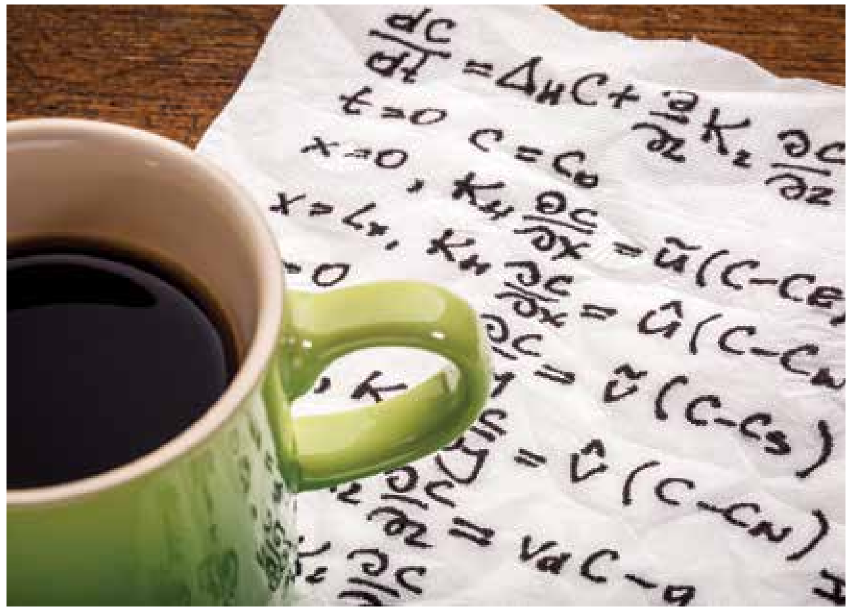
A numerical problem of the past

In the 1950s, when FORTRAN was just being developed, Turing had only just proposed his test and computers were the size of a room, it was nearly impossible for scientists to find numerical answers to engineering and physics questions. Given the very limited computing resources available at the time, the solution was to break continuous problems into their component parts onto local meshes. This situation led to the development of mesh generation that has become an art form over complex domains. Various finite methodologies have evolved since the 1950s.

The finite difference method is used to approximate the derivatives of continuous functions with finite difference equations. However, the basic notions of calculus show how the difference should tend to zero rather than to a small but finite error. Naturally, these differences compound when calculations are large and not particularly well-behaved. At the time when computers were themselves relying on inaccurate floating point approximations, round-off errors were adding to the differences between the numerical calculation and the actual value of the derivative. The most noteworthy problem was not necessarily that the calculations were approximate, but that they were unreliable. Sometimes it was difficult for scientists to tell when they obtained an approximately precise result or when the opposite was true, that the result was not even in the same ballpark as the value for which they were searching. This led to an ingrained caution against 'ill-conditioning'. Simply stated, ill-conditioning is the accumulation of round-off errors on finite precision computers that can render calculations meaningless. Computer scientists devised methods to control rounding errors, and develop extended precision arithmetic so that, at the end of a calculation, the results are reliable to at least 'n' significant digits.

The finite element or finite volume method on the other hand, is splitting a surface or a volume into component parts and assigning a finite function – onto a mesh – to each of these pieces. In other words, the mathematical treatment involved applying a function to model the behaviour of each piece. However, most functions used for modelling mathematical surfaces are continuous functions. In advanced calculus such functions can be understood through Taylor series, which sum up the derivatives of a function to obtain an approximation

‘I demonstrated that by moving points in space as exact differentials with source terms, no artificial physics needed to be introduced for time dependent problems’



approaching the initial function as the number of derivatives approaches infinity. The problem is that when using a Taylor series on a surface with a finite radius, the series can converge to the initial function inside the radius but may be very far from the function outside this boundary. This situation hides a trap similar to that of the finite difference method. For smooth functions, there are an infinite number of derivatives, and therefore the Taylor series has an infinite number of terms which can cause errors. The errors arising from the remaining terms of the Taylor series expansions are known as truncation errors; these should go to zero as the mesh spacing goes to zero, but this does not happen in reality. Additionally, the unknowns come from the infinite tail of the series and not from the first few terms at the front. Cyclic functions such as the sine and cosine are particularly nice because their derivatives repeat at fixed intervals, making the problem easy to solve. However, functions with great value variations between one point and the next cannot be approached through generalising the first few derivatives. It would then be left to the engineer or physicist needing the computation to check by pen and paper whether the calculation is correct. This is often impossible and, moreover, it defeats the purpose of using a computer.

The finite difference and mesh methods described so far have direct applications in physics and engineering. As you’ve gathered by now, Dr Kansa’s complex work often faced him with exactly these problems on a daily basis. He knew scientists often had to sacrifice the accuracy of the physics to make calculations approachable through the available numerical methods. He felt that since physics had to be adapted to the computational methods, it became slightly artificial. Artificiality happened because the functions known to behave well are only a few compared to the number of functions that truly model the behaviours of some systems. When faced with such problems in the past, scientists had to approximate complex behaviours with slightly unsuitable functions, which were guaranteed to work with the available numerical methods but were not necessarily the best modelling option. Scientists relied on brute force to obtain reliable numerical results by using massively parallel computers, relying upon arcane numerical methods designed in the 1950s.

From astrophysics to explosions and cancer growth

Examples illustrating the problems of approximations start in the two dimensional plane and extend to the curse of dimensionality, a phenomenon occurring in higher dimensions. An irregular, snaking line in the plane is a visual representation of a spline, a piece-wise row of mathematical functions held together by knots. Knots are points where the functions patched together have enough derivatives to ensure the existence of a path from one component function to the next. Any spline passing through more than three points in the plane is difficult to model because the points at the end of each separate function oscillate too much due to numerical approximations. When this problem is extended to more than one dimension, it amplifies proportionally to the number of dimensions – and the errors are not simply due to computational methods. Sometimes, the input of a function can be a value obtained after a measurement, for example the length of an airplane wing. The function modelling the behaviour of the wing inside an air current may be overly sensitive to the initial measurement error, in such a way that its output errors grow in the second decimal digit even if the initial error was in the tenth decimal digit; the output error in this case would be 8 orders of magnitude larger than the input error. When a function or process such as solving systems of equations is accumulating too many errors too fast, the problem is called ill-conditioning. For some cases, this problem becomes exponentially worse as the degrees of freedom of the system increases – a phenomenon called the curse of dimensionality.

For example, the quantum mechanical calculation of the electronic structure of H_2O is a 9-dimensional problem. With 10 discretisation points per dimension, the total 1 billion is considered very sparsely discretised. Sometimes, the system has sparse matrices – with many points where the action is zero – however, the zeroes still need to be calculated, thus increasing the calculation time. Naturally, the problem is even more difficult when the matrix is dense, meaning that it has a lot more non-zero entries.

Dr Kansa started looking for a solution to these cases, a solution that would make his and his colleagues’ lives easier and their calculations more accurate. ‘I became interested in highly convergent meshfree computational methods because the standard methods changed the physics to conform to the numerics, rather than changing the numerics to conform to the physics. I demonstrated that by moving points in space as exact differentials with source terms, no artificial physics is needed to be introduced for time dependent problems’, Dr Kansa explains.

Dr Kansa’s work can be applied to many fields, from astrophysics and quantum mechanics, to plasma fusion, cancer growth, and shocks and explosions. For example, shocks and explosions are problematic to compute out of the theory. Firstly, this is because the theory is that of Navier and Stokes, incomplete in this area. Secondly, the calculations may become singular and therefore result in infinities, which are certainly not observed in practice. The solution is better numerical methods, as Dr Kansa observed: ‘The main idea in our recent work is that numerical methods of the 1950s were adapted to very primitive computers and have not evolved since then. The excuse that meshfree methods suffer from “ill-conditioning” is obsolete, and fast extended precision methods now exist. It seems counter-intuitive that global or widely banded methods based on C^∞ functions requiring extended arithmetic precision is superior in both accuracy and execution speed on a specific computer. Exponential convergence always wins over the slow convergence rates of finite methods. Presently, these C^∞ radial basis functions appear to be suited ideally for high dimensional problems.

C^∞ radial basis functions are global in nature yield either full or broadly banded systems of linear or nonlinear equations. The infinity sign shows that such functions belong to a class of functions with an infinite number of derivatives, otherwise known as smooth functions. Dr Kansa extended the class of radial basis function to include finite jump discontinuities in the normal propagation direction, but is infinity smooth in the tangential directions. C^∞ functions converge exponentially, depending upon the shape ratio defined as the ratio of the average shape parameter to the average minimum distance. The larger the ratio becomes, the faster is the convergence rate. In contrast, standard linear finite difference and finite element schemes only converge at the typical quadratic rates.

C^∞ functions are suitable for many types of equations – integral, partial differential, integrals, or integro-partial differential equations. Moreover, highly dimensional systems are reduced to one-dimensional problems due to the equivalence between the location and value of the points in the original governing equation and the points of the C^∞ functions. Since C^∞ functions only depend on the distance to a centre, they can work in the flat Euclidean, spherical polar geometry, or with geodesics such as those used in general relativity. Changing the norm – the notion of the distance in the space – makes radial basis functions versatile and applicable to most computational physics problems.

In addition, Dr Kansa found another advantage of meshfree C^∞ functions. For time dependent problems, one can find a local velocity at each evaluation point that transforms a complicated nonlinear equation with source terms into an exact differential for the expansion coefficients. The time dependent expansion coefficients are exactly solved. Any redistribution of evaluation points is rigorously constrained to conserve mass, momentum components, and total energy without violating the basic principles of physics.

A powerful numerical method offers a viable way to calculate computationally intensive problems in physics and engineering, without the errors plaguing finite volume and element methods

Radial basis functions have many advantages. Whereas the finite methods can only use the first few terms of the Taylor series and become worse as the number of dimensions increases, radial basis functions have been shown to exponentially converge to the original function depending on the dimensionality of the problem and the shape ratio parameter. Since radial basis functions are continuous, their derivatives are not interrupted at the traditional mesh boundaries seen in finite methods. Finite methods have compact support, or alternatively, the value of the functions outside the mesh boundary is zero. In his recent work, Dr Kansa found a formula that models solutions on the interior space and on its boundary as a sum of a radial basis functions and a set of time-dependent expansions coefficients with a forcing function. To extend this solution method to higher dimensions, he offers a second formulation in which the boundary, interior, and time dependent problem are cast into a ‘fuzzy’ global minimisation problem that works for both well-posed and ill-posed problems. The system of equations can be shown to be spectrally equivalent with the initial problem, and therefore the solution is mathematically correct. Such systems of equations can sometimes still result in some ill-conditioning arising from round-off errors due to the limited precision of floating point computation. Presently, computer chip manufacturers are concerned with providing hardware for social media and gaming devices, not for scientific computing. Consequently, alternative software remedies of varying quality are available. Dr Kansa and Pavel Holoborodko showed applications of their extended precision arithmetic in their recent work. The method can use multi-precision tools, eigenvalue decomposition, and can find global zeros of a function, displaying impressive numerical precision when compared to traditional methods.

Dr Kansa’s research opens new paths towards better numerical methods, yet challenges still remain. One of the greatest challenges is the necessity to divide the calculations to massively parallel computer systems, which would greatly reduce the time for each computation. But Dr Kansa promised to continue his efforts in that direction: ‘My next research area will be exploring new methods to reduce the computational time to solve important multi-dimensional equation systems.’

Meet the researcher

Dr Edward Kansa
Convergent Solutions,
Livermore
California, USA

Dr Edward Kansa received his PhD at the Vanderbilt University in 1972 in many-body quantum theory, after which he continued to work in applied math and physics modelling problems with the U.S. Bureau of Mines and Lawrence Livermore National Laboratory from 1980 to 2004. Dr Kansa held teaching positions at the Department of Mechanical and Aerospace Engineering of University of California and the Department of Physical Sciences of Embry-Riddle Aeronautical University. The Kansa meshfree method has wide applications in engineering and physical science for differential equations in computationally intensive contexts. Kansa authored over 120 papers and received over 4800 citations.

CONTACT

E: edwardjkansa@netzero.com
W: www.researchgate.net/profile/Edward Kansa

KEY COLLABORATORS

Pavel Holoborodko, Multiprecision Computing toolbox, Kanagawa, Japan.
Alexandre I. Fedoseyev, Computational Fluid Dynamics Corp., Huntsville, Alabama, USA
Juergen Gieser, Ruhr Universitaet, Bochum, Germany
Levan Ling, Hong Kong Baptist University, Hong Kong
Yiu-Chiug Hon, City University of Hong Kong, Hong Kong
Antonio Fererra, University of Porto, Oporto, Portugal
Nicolas A. Libre, Missouri Science and Technical University, Missouri, USA
Anita Wong, Open University of Hong Kong, Hong Kong
Efim A. Galperin, University of Quebec at Montreal, Montreal, Quebec, Canada
Athena Markogolu, University of Portsmouth, Portsmouth, UK
Scott Sarra, Marshall University, Hunington, West Virginia, USA
James Wertz

FUNDING

National Science Foundation (United States)
SBIR Small Business Innovative Research, division of the National Science Foundation

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The challenges of complexity

The Department of Electrical Engineering at the United Arab Emirates University provides world-class education while conducting cutting-edge research in a number of areas. Through close collaborations with major industrial partners, they provide solutions and advice for real-world problems.

A car which drives you from home to work at the touch of a button, with no intervention required. An aeroplane which can land itself in the middle of the thickest fog, without the hand of a pilot at the controls. A robot submarine which can travel for weeks under the polar ice, with nothing more than a vague command to explore the area. Only a few short years ago these would have been dismissed as pure science fiction, but today all of them are real.

The rise of autonomous vehicles, (drones, if you will), is the most visible change that has been brought about by rapid advances in the field of automation. Thanks to vast increases in computing power and program complexity, it is possible for a computer to take input from a number of sources and then decide how to achieve its goal – all without human intervention. Robot cars are obvious beneficiaries, but complex automation finds its way into manufacturing, toll booths, ship stabilisation and more.

The down-side of complex automation, of course, is that there is a far greater scope for something to go wrong – and no amount of engineering can completely prevent faults from occurring. Automated systems thus need to be able to detect, and correctly react to, faults before they affect the entire process – this is known as Fault Tolerant Control, (FTC).

Fault tolerant control relies on the existence of diagnostic modules, which provide a continuous stream of information on the health and status of the system they are monitoring. When a fault occurs, diagnostic modules inform the central automating system, which can then compensate for the change – thus keeping conveyor belts running and aeroplanes in the sky.

What are the requirements for a diagnostic module? It needs to be fast enough to respond to changes in the system, it is no good knowing that the brakes have failed after the car has hit the post-box, after all. It must also be able to accurately diagnose, to determine just what the problem is. This is a surprisingly complicated requirement, as it often requires the module to make a best guess as to what is happening in the face of conflicting information. Accurate diagnostics modules use comprehensive knowledge models of the system combined with complex decision-making algorithms to make sense of these situations.

Quis creat custos?

The development of these systems requires significant expertise, and this is where scientists such as Professor Hassan Noura come in. A well-known researcher in the field of fault tolerant control, his expertise has been called upon for fields ranging from helicopters and microchips to fuel cells and unmanned aerial vehicles. Currently the Chair of the Electrical Engineering Department at the United Arab Emirates University, he began his research career in 1990 as a PhD student at Lorraine University, France. There he was one of the first researchers in France to work on fault-tolerance in automated systems, using a heating system which could adapt to failures on the fly. His career rapidly progressed, with an Associate Professorship at Lorraine University being quickly followed by a full Professor position at Aix-Marseille University. He moved to the UAE in 2007, before taking up the Department Chair position in 2011.

Throughout this time he has specialised in the development of fault tolerant control systems for a various problems, often in collaboration with industry partners. Automation has spread throughout many facets of modern industry, and the basic approach to fault-tolerant design is inherently flexible, allowing the same paradigm to be applied to many different areas.

Indeed, renewable energy in remote locations has become a minor focus of the group, with research being performed on diagnostics systems for fuel cells, wave energy convertors, and solar plants. Fuel cells, which convert chemical energy directly into electricity, are often used in remote situations for power generation. Collaborative research between UAE University and the Japan Co-operation Centre, Petroleum has begun with the aim of developing diagnostics modules for fuel cells, particularly in high-temperature situations – a natural concern for a desert state. A small-scale wave energy generator has recently been installed at the university, and will act as a basis for work both for the control and diagnostics group and for others in the electrical engineering department. Renewable energy is a surprising choice in the UAE, which is one of the world's largest exporters of petrochemicals, but represents a general move by the UAE over the last few years to diversify their technology and economic base.

Flying free

But Professor Noura's main interest lies not in the ocean, but in the skies. At his urging the United Arab Emirates University has recently launched a dedicated facility for work on Unmanned Aerial Vehicles, where students and researchers can develop new methods for both autonomous control and fault tolerance. The group focuses on rotary-winged UAVs, such as quadcopters, (the four-rotor drones often seen in your local park), or octocopters (their eight-rotor big brother). The UV Lab Family, as they call themselves, focus their research on the design of both fault-tolerant control components and the associated software – with the ultimate goal of designing a UAV which can remain flying in the face of multiple failures. As a plummeting UAV can do significant damage to property, (damage which is often specifically excluded from insurance policies), being able to prevent this is a valuable goal to have.

In a world of complex automated systems, what happens when a part breaks? Less than you would think, thanks to the work of researchers such as Professor Noura.

Their expertise in these areas has led to a number of contacts with industrial aerospace firms, as it can be directly applied to the more traditional type of aeroplane as well. The majority of modern aeroplanes use 'fly-by-wire' controls – in which electrical signals, rather than mechanical pulleys, convert pilot actions into movements of the control surfaces. These systems are lighter and allow for automated flight stabilisation, but are more susceptible to the failure of control modules. As such, diagnostics modules and fault-tolerant systems are a necessity for modern aeroplane design, particularly when working with high performance fighters which may be damaged in combat. Part of Professor Noura's work is done in collaboration with Dassault Aviation, manufacturers of various aircraft including the hypersonic Mirage and Rafale, to create systems which can handle failure at high speeds and low altitudes.

These developments are also applicable to civilian craft, a further collaboration with Eurocopter involves improvements in diagnosing changes in helicopter drive-trains. Failures of the drive-train, which couples the engine to the rotor, have led to numerous crashes – and thus early identification of discrepancies in the system can allow preventive maintenance before catastrophic failure.

The fields of automation and automated process control have taken a long road to reach their current state. Shall we start in the whistling of steam engine governors from James Watt's time, or the gentle glow of the failure-prone vacuum tubes running the first automatic telephone switchboards? Compare this to today, in which factories can run for months without human intervention, and autonomous aircraft can patrol the oceans for weeks. The expansion of the power and reach of automation requires a corresponding growth in the ability to control these systems under imperfect conditions. It is this next stage, the creation of truly adaptive, fault tolerant systems, where researchers such as Hassan Noura are leading the way.

Researcher Profile

Professor Hassan Noura
Chair, Department of Electrical Engineering
United Arab Emirates University

Professor Hassan Noura is the Chair of the Electrical Engineering Department at the United Arab Emirates University. With a PhD from Lorraine University, France, in 1993; followed by Professorships at both Aix-Marseille University, France and UAE University; his career has been highly international both in location and collaboration. Professor Noura has had a long and distinguished career in the field of fault-tolerant control systems, developing automated systems which can work in the presence of failed components or errors. This work is applicable to a number of fields, and he has performed a number of joint projects with world-leading industry partners. He is also responsible for the development of the first unmanned vehicle laboratory at UAE University. He teaches a number of subjects involving automation and control, and has supervised 12 PhD students. During his career, Professor Noura has been the author of one book, three book chapters, and numerous journal and international conferences articles.

CONTACT
E: hnoura@uaeu.ac.ae
T: (+971) 3 713 6582
W: http://www.eng.uaeu.ac.ae/en/profile/profile.shtml?email=hnoura%40uaeu.ac.ae

COLLABORATORS
Dr. Sulaiman Al Zuhair, UAEU, Chemical and Petroleum Engineering Department
Dr. Francois Bateman, French Air Force Academy, France
Prof. Ahmed El Hajjaji, The University of Picardie Jules Verne, France
Dr. Abbas Fardoun, UAEU, Department of Electrical Engineering
Prof. Mustapha Ouladsine, Aix-Marseille University, France
Dr. Jean-Christophe Posart, Lorraine University, France
Dr. Abdel-Hamid Rabhi, The University of Picardie Jules Verne, France
Prof. Dominique Sauter, Lorraine University, France
Prof. Didier Theilliol, Lorraine University, France
Dr. Addy Wahyudie, UAEU, Department of Electrical Engineering
Prof. Youmin Zhang, Concordia University, Canada

FUNDING
UAE University Program for Advanced Research
Japan Cooperation Center, Petroleum (JCCP)
Dassault-Aviation
Abu Dhabi Autonomous Systems Investments (ADASI, UAE)
Abu Dhabi Police

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Unmanned Vehicle's Lab

http://faculty.uaeu.ac.ae/hnoura/uvsl/index.html

A novel electric current simulator in the human brain

Dr. Shoji Hamada is an Associate Professor and a research scientist interested in studying and developing computational tools for the analysis of electromagnetic fields in anisotropic conductive media, with wide implications in biomedical engineering applications.

Can you provide our readers some background and an outline of your research?

My specialty is the development and conceptual design of numerical calculation methods for fields in the human body. The voxel-based indirect boundary element method (IBEM) and the voxel-based method of moments (MoM) are examples of such numerical field calculation methods.

Biological neural activities generate electric currents in the body, voltage differences on the skin surface, and magnetic fields around the body. By quantitatively calculating the quantities caused by each unit of neural activity at every possible position, for example, we can noninvasively estimate the distribution of brain neural activities by analysing a measured brainwave and magnetic encephalographic signal with inverse calculation techniques. Note that an inverse calculation needs preliminary forward calculations like these.

On the other hand, when electric, magnetic, and electromagnetic fields are applied to a patient, they induce electric fields and currents in the body. For example, transcranial magnetic stimulation applies external magnetic fields to the human head to induce electric currents in the brain for symptomatic treatment, and a defibrillator is used to apply contact currents to the human body to stimulate the heart and re-establish effective rhythms. By quantitatively calculating the actual current distribution, we can improve the performance and effectiveness of these devices.

In order to improve calculation accuracy and reliability, it is important to consider the following key techniques: [i] using "tailor-made" numerical human models derived from personal MR images, [ii] considering anisotropic conductive properties of biological tissues such as nerve fibre bundles, and [iii] developing or improving a field calculation method suitable for [i] and [ii].

How do you use data from magnetic resonance imaging (MRI) in your research?

The MRI technique noninvasively provides internal structural information of organs, and the numerical human models developed from the MR images are very good replicas. In particular, an accurate personal model can be produced from MR images, which are most accurate for an individual.

The diffusion tensor imaging (DTI) technique available lately is a variant of MRI. The diffusion tensor can be approximately converted to an electric conductivity tensor that represents the anisotropic conductivity of the biological tissue. Therefore, by using MRI and DTI, we can develop numerical human models that have both the structural and conductive information derived from the body.

MR images are provided as a stack of pixel pictures, which are called voxel data, and are equivalent to a three-dimensional, equal-interval, orthogonal coordinate grid. Thus, by using voxel models and field-calculation methods suitable for voxel model analyses, we can efficiently perform numerical field analyses.

Can you provide us more detail on voxel-based static MoM and related method voxel-based IBEM?

The voxel-based static MoM and voxel-based IBEM are low-frequency electric-field calculation methods designed to be suitable for voxel model analyses. The voxel-based IBEM can analyse large-scale voxel models having structural information derived from MRI. In comparison the voxel-based static MoM can analyse voxel models having both structural and conductive information derived from MRI and DTI, respectively.

Standard IBEM is designed to calculate the currents through isotropic tissues. The voxel-based MoM technique enables us to numerically calculate electric currents flowing through anisotropic conductive tissues such as nerve fibre bundles. By visualising the calculated current distribution, we can observe them. My recent conference paper describes how we developed and verified the voxel-based static MoM.

What alternative numerical calculation techniques are there for analysing electric current flowing through anisotropic tissues such as nerve fibre bundles?

Numerical field calculation methods that can also address anisotropy are finite difference methods (FDM) and finite element methods (FEM). In comparison the advantage of the combined use of the voxel-based static MoM and voxel-based IBEM is as follows:

Let us assume the voxel model to be analysed is composed of D × D × D voxels, for simplicity. A simple estimation of calculation time and computer memory indicates a D^2 dependency for the voxel-based IBEM using the fast multipole method (FMM). This dependency comes from IBEM using surface elements. On the other hand, the dependency of the FDM, FEM, and voxel-based static MoM is D^3, because these methods are practically based on volume elements. These dependencies suggest that the voxel-based IBEM is suitable for large-scale model analyses. Because voxel-based static MoM is suitable for use with the voxel-based IBEM, their combined use would be the best choice.

What applications except for electro/magnetoencephalography can your method be useful for?

The numerical calculation technique can help us to improve electric devices directly affecting the body, like defibrillators and electro-surgical knives, because design parameters of these devices could be effectively optimised by running well-organized numerical simulations. The parameters that could be optimized are, for example, shape, size, position, and the number of electrodes and coils; intensity, frequency, and wave form of electric power sources.

Computing electric currents by considering anisotropies in the brain

A new voxel-based computational method enables the high-speed and large-scale simulation of electric current flowing through anisotropic conductive tissues such as nerve fibre bundles by using biological voxel models derived from medical images.

COMPUTING ELECTROSTATIC FIELDS

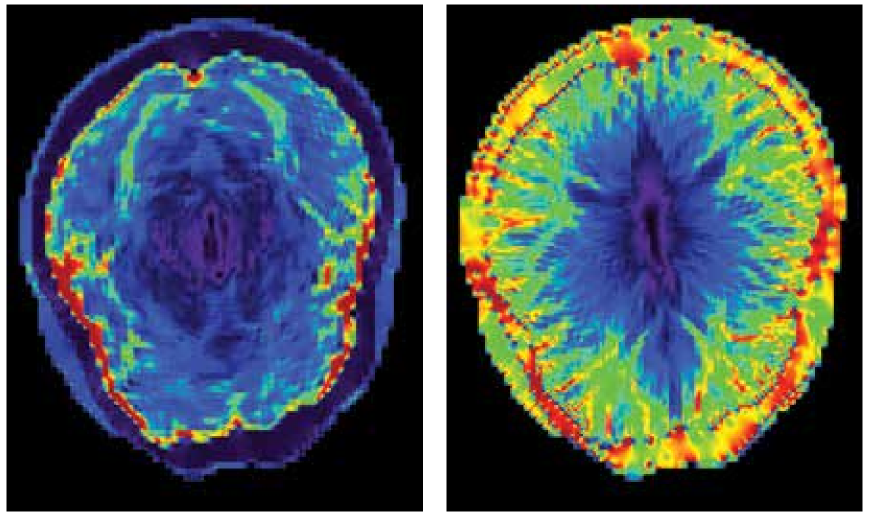
Dr. Shoji Hamada is an associate professor at Kyoto University, Japan, and specialises in computational electromagnetics and electrical engineering. Throughout his career he has developed a range of computational methods and models for the analysis of electromagnetic phenomena in the human body and in dielectric media. We look at his recent work and conference paper "Electrostatic Field Analysis in Anisotropic Conductive Media Using a Voxel-Based Static Method of Moments".

Hamada has developed a novel computational method that can analyse the electrostatic fields and currents in anisotropic conductive media such as nerve fibre bundles in the human brain. This method is designed to analyse a cubic voxel model that is a stack of two-dimensional pixel arrays (i.e. picture data). The structural information of a voxel model is derived from magnetic resonance imaging (MRI) data, and the anisotropic conductivity tensor of each voxel is derived from diffusion tensor imaging (DTI) data.

Although typical field calculation methods utilize volume elements to address anisotropic conductivities, this method adopts surface elements that emulate volume elements. This choice enables the method to be used concurrently with the voxel-based indirect boundary method (IBEM), which is another field calculation method that uses surface elements. The voxel-based IBEM can perform high-speed analyses of large-scale 'isotropic' conductive models. Thus the combined use of this method with the voxel-based IBEM provides improved computing performance in analysing composite media composed of both isotropic and anisotropic conductors.

MAKING REALISTIC VOXEL MODELS FROM MRI AND DTI DATA

MRI is a diagnostic technology widely used in contemporary medicine for its capacity to measure and image minuscule detail. This technology works by using a superconducting magnet to create a strong magnetic field that passes through the patient. The field aligns the spinning hydrogen protons, present in water in the body, along the same direction as the field, thus making the patient virtually transparent for observation. Then a radio wave is pulsed into the target organ to knock the protons out of the regular array. When the radio wave is turned off, the protons re-align with the magnetic field, and as they do so, emit their own radio waves which are detected by instruments inside the machine. These waves carry a signature of the tissue type and injected contrast dye and create the contrast between organs and tissue types.



Calculated current density ***J*** and electric field ***E***.

To obtain reliable calculation results, it is important to make human voxel models as realistic as possible. Thus we utilize MR images to produce a human voxel model. The MRI technique noninvasively and experimentally provides the internal structural information of human organs, and the voxel models derived from MR images are very good replicas of real bodies. The DTI is a variant of the MRI, and the diffusion tensor can be approximately converted to an electric conductivity tensor that represents the anisotropic conductivity of the biological tissue. By using MRI and DTI data, we can develop voxel models that have both structural and conductive information experimentally derived from an original human body.

In particular, an individual personal model can be produced from personal MRI and DTI data. This is of course the most accurate model of a person. By using such models we can substantially improve the reliability of the calculated electric fields and currents in the model. Such high accuracy is desired for brain-related medical applications in particular.

DETAILS OF DEVELOPED VOXEL-BASED METHOD

In more detail, this new numerical method is a voxel-based static method of moments (MoM). A voxel is a three-dimensional pixel that acts as a small volume element comprising a larger computer model, whereas "static" refers to the electrostatic and quasi-electrostatic fields which are the targets of the calculation. The method of moments is a widely used tool for solving integral equations to compute electromagnetic fields in numerical models – in this case, voxel human models derived from MRI and DTI data. In his paper, Hamada used his voxel-based MoM to analyse an anatomically exact computer model composed of a three-dimensional array of cubic voxels constructed from imaging data. "Usually, MR images are provided as voxel data and are equivalent to a three-dimensional equal-interval orthogonal coordinate grid", Hamada said.

The voxel-based IBEM and MoM utilize surface elements, and an element is defined on a square voxel wall between two voxels having different values of conductivity. This definition makes the data structure simple and efficient to handle. In particular, the simple structure enables the IBEM and MoM to straightforwardly utilize both the fast multipole method (FMM) and the fast Fourier transformation (FFT) algorithms. These algorithms dramatically speed up the calculation speed and increase the available number of unknowns.

In addition, using this type of element guarantees a calculation accuracy comparable with that of the finite difference method, which is widely recognized as a practically useful approach. On the other hand, the element definition makes the model shape suffer staircase-shaped errors. The voxel-based IBEM and MoM are designed to address this weak point by using high-resolution and large-scale models that can be handled by using the FMM and FFT. The voxel-based MoM has previously handled up to 284 million unknowns on a personal computer with 64 GB of main memory.

The voxel-based MoM emulates a volume element by using six surface elements defined on six surfaces of a cubic voxel. These six elements represent the distribution of polarization charges in the volume. 'In a conductive medium, the sum of polarized charges inside any closed region is zero', Hamada explained. 'However, the standard IBEM cannot numerically satisfy this relationship in anisotropic conductive media. The voxel-based MoM can numerically satisfy this relationship even in anisotropic conductive media because we designed it to satisfy this relationship by adding a constraint to the basic equations'.

RESEARCH IMPLICATIONS

These computational methods are crucial for researching and developing biomedical engineering applications such as electro/magnetoencephalography, electric/magnetic stimulation, and exposure assessment for electromagnetic fields. A typical application of the field calculation technique is the forward calculation preliminarily required by the inverse calculations for electroencephalography (EEG) and magnetoencephalography (MEG). EEG and MEG reveal the distribution of neural activities in the brain by analysing the measured brainwave and magnetic encephalographic signal using inverse calculation techniques. The improvement in forward calculation accuracy improves the reliability and resolution of analysed neural activities.

Moreover, transcranial magnetic stimulation (TMS) is used for therapeutic reasons and to measure brain activity for diagnostic purposes. The potentially harmful effects of TMS can be avoided because they can be simulated and understood in advance. Electrical devices that directly affect the body, such as defibrillators and electro-surgical knives, can also benefit greatly from this method. Defibrillators are used to impart an electrical current across the heart to return it to normal rhythm, and electro-surgical knives are used to cut tissue during surgery. Hamada informs us that "numerical simulations can be used to optimise design parameters such as shape, size, position, and the number of electrodes and coils; and the intensity, frequency, and waveform of electric power sources".

This research is important because "Anisotropic conductivity is exhibited by a variety of biological tissues, for example, bones, muscles, and nerve fibres', said Hamada. The voxel-based IBEM and MoM are designed to suit isotropic and anisotropic media, respectively. Overall, the analysis works best if voxel-based IBEM is used in conjunction with voxel-based static MoM. It is the combination of these methods that results in the greatest advantage. The resulting increase in computing performance will contribute to analyses of finer-resolution and larger-scale models and obtain better accuracy and reliability. 'Our goal is to prevent harmful effects to the human body caused by electric, magnetic, and electromagnetic fields, and to effectively utilize their beneficial effects', Hamada said.

Researcher Profile

Dr. Shoji Hamada
Department of Electrical Engineering,
(Biological Function Engineering)
Kyoto University

Dr. Shoji Hamada is Associate Professor at Kyoto University, Japan, and specialises in computational electromagnetics, electrical engineering, electrical discharges, and electric field calculations, with over 50 published contributions to the field of physics. He received his Ph.D. in electrical engineering from the University of Tokyo 1992. Afterwards he worked with the Tokyo Denki University 1992-1997, and has been a lecturer since 1997 at the Department of Electrical Engineering, Kyoto University, returning to where he completed his B.S. degree. He is a member of IEEE, IEEJ, and JSST.

CONTACT
T: +81 75 383 2230
E: shamada@kuee.kyoto-u.ac.jp
W: http://researchmap.jp/read0027006/?lang=english
W: http://bfe.kuee.kyoto-u.ac.jp/en/research05.html
W: http://www.kuee.kyoto-u.ac.jp/~shamada/index_e.html

FUNDING
Japan Science and Technology Agency (JST)
Japan Society for the Promotion of Science (JSPS)

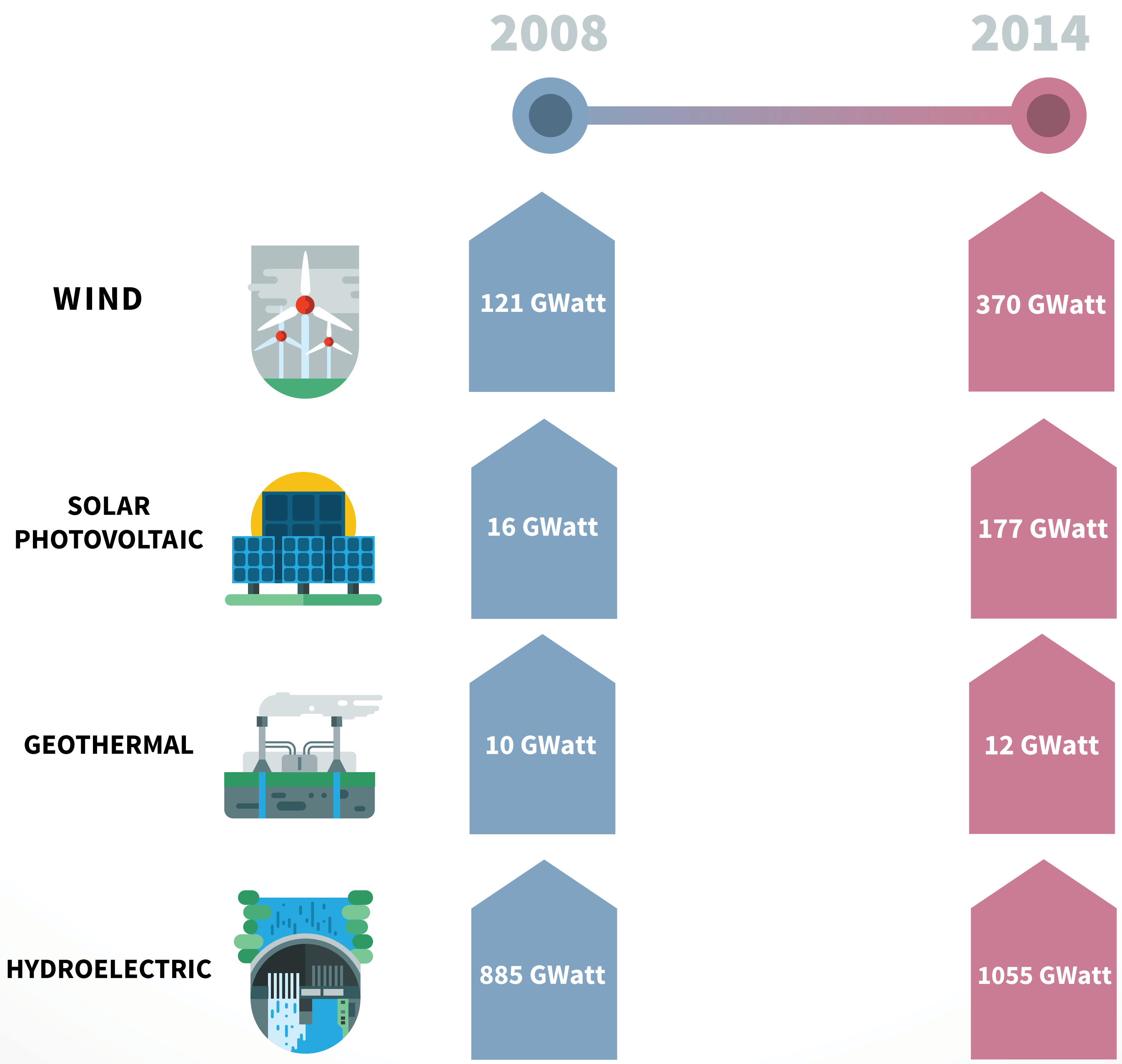
CLEAN ENERGY TECHNOLOGIES FOR THE FUTURE

Burning up the earth's underground energy-rich resources to power our world is an innovation that dates back to the industrial revolution in the late 18th century. Despite the deleterious effects of global warming that we are already experiencing, we are now spewing more carbon dioxide into the atmosphere than ever before – an estimated 40 billion last year alone. The heat-trapping properties of carbon dioxide have led to a 1 °C rise in the global temperature, with 2015 being the hottest year ever on record. World leading scientists are warning that having surpassed this milestone, we are now entering into 'uncharted territory', with the most catastrophic climate consequences yet to come. However, if we can start to drastically reduce the volume of carbon dioxide we release into the atmosphere, while also actively removing it from the air, there may still be hope that we can avoid a major climatic disaster. >

> Huge progress has been made in developing clean energy technologies in recent years. However, only about a quarter of the world's electricity is generated from renewable sources, and this fraction is much less when looking at our entire energy consumption (electricity, transport and industry etc.), so there is much work needed to be done. Generating electricity from solar and wind are two extremely promising technologies, however, both yield an intermittent energy supply (only generating electricity when it's windy or bright out, respectively). Therefore, in order to maximise their efficiency, we need to develop new ways of storing the electricity generated from these sources. In this section we showcase the latest innovations in energy storage technology, in a research project led by Professor Maria Forsyth. Professor Forsyth and her team are leading the change by developing sodium based batteries that are viable for integration with the future renewable energy grid.

One source of clean energy that has not yet been realised on Earth is nuclear fusion. Fusion is the process through which or sun produces energy, fusing hydrogen nuclei together to form helium, releasing energy in the form of photons. This excess energy arises due to a slight loss of mass that occurs during this process, which is converted into energy as described by Einstein's famous formula E = mc2. Achieving controlled nuclear fusion on earth could help to solve the worlds energy crisis, by offering a new carbon-free alternative to fossil fuel combustion. The second article in this section showcases the research of Dr Scott Hsu and Dr F. Douglas Witherspoon, who are leading a multi-institutional research programme that is currently developing a novel approach to fusion power, or so called plasma-jet-driven magneto-inertial fusion (PJMIF).
As promising as these renewable energy technologies are, human beings will unfortunately continue to burn up fossil fuels for the foreseeable future. Recognising this truth, Sofiane Zalouk and Johan Rey are both working on improving the sustainability of industrial boilers used to generate electricity. In the final article of this section, we discuss their novel carbon capture technology that can trap up to 90% of the carbon dioxide emitted from intermediate boilers. Preventing this greenhouse gas from being released into the atmosphere, and either storing or reacting it to form organic compounds, represents a huge leap along the path of climate change mitigation.

GLOBAL ELECTRICITY PRODUCTION CAPACITY OF RENEWABLE ENERGY SOURCES: 2008 VS 2014



RENEWABLE ENERGY GETS A BOOST FROM SODIUM BATTERY TECHNOLOGY

Professor Maria Forsyth and Dr Patrick Howlett are leading a project funded by the Australian Research Council to develop sodium-based energy storage technologies to bolster a future renewable energy landscape. Sodium-based batteries will give renewable energy a much needed boost in the replacement of fossil fuels.

Lithium gives way to a sodium revolution

Renewable energy is steadily replacing the world's entrenched reliance on fossil fuels, which continue to release carbon into the Earth's atmosphere. Renewable energy plants composed of arrays of wind turbines or solar panels, for instance, are clean and sustainable alternatives, but they have a downside – they cannot function continuously because they rely on favourable climate and weather conditions. This is where battery technology comes in to work with renewable energy sources. As a wind turbine produces more energy in windier conditions, that energy can then be stored in batteries. The energy can then be supplied to the grid when needed, when weather conditions are not windy or sunny enough to meet the energy demand.

The last few decades have seen concentrated developments in lithium-ion battery technology, but lithium is by no means the only element that can be used for electrical energy storage. Sodium has been identified as a successor to lithium for important reasons. One reason is that sodium is orders of magnitude (hundreds or even thousands of times) more abundant than lithium. In addition, more than 70% of the world's lithium ore comes from only a few locations in South America. These factors lead to instability in the lithium market and have already caused problems with availability and supply. With sodium also being a safer substance, sodium-based battery technologies are regarded to be a supporting pillar for future energy systems.

Professor Maria Forsyth and Dr Patrick Howlett at the Institute for Frontier Materials (IFM), Deakin University are leading researchers in battery technology and electrochemical devices. Their work focuses on studying the dynamics of charge transport in electrolytes and metal-electrolyte interfaces. The team are currently conducting research into sodium-ion conducting electrolytes for battery technology, funded by the Australian Research Council (ARC). The IFM can facilitate the highest quality energy storage and materials research due to its Nuclear Magnetic Resonance (NMR) Facility, Microscopy and Characterisation Suite, and electrochemistry laboratories. These facilities attract an outstanding calibre of researchers that are well placed to perform research at the highest level.

The current state of the art in sodium-based research focuses on developing and testing sodium electrolytes required in batteries. Presently, sodium-based batteries are limited by high operation temperatures, roughly 300 °C, and short lifetimes, making them insufficient for mainstream use. Professor Forsyth and Dr Patrick Howlett, along with Michel Armand from CIC Energigune (with funding from the ARC) are developing high conductivity, ambient temperature sodium electrolytes in order to push past these limitations, towards making batteries that are viable for integration with the future renewable energy grid.

The initial goal of the project is to diligently design experiments and devices, which will set the stage for a successful outcome. Research and development will include the characterisation of sodium electrolytes to probe their properties and electrochemical performance. A parallel goal is to study the molecular properties of sodium electrolytes in order to better understand sodium ion dynamics and chemical speciation. These goals will precede the production of battery prototypes that fall into three main categories: ambient temperature sodium metal batteries (necessary for environmental conditions that the batteries will ultimately operate in), sodium-ion batteries with improved performance, and sodium-based hybrid supercapacitors (capacitors that can store a lot of energy).

Sodium-based batteries

A simple battery is made up of two electrical terminals called an anode and a cathode, between which an electric current flows through a liquid electrolyte from cathode to anode. Cutting edge sodium technology usually adopts a molten sodium anode and a molten sulphur cathode. Another battery type, called a ZEBRA battery, comprises a beta-alumina ceramic electrolyte and a nickel chloride cathode. Two of the main reasons that sodium technology is still in its infancy are that these types of batteries experience substantial manufacturing problems, and in terms of application are only suitable for large devices that are used continuously. This shows why lithium-based technology initially took off rather than sodium-based technology, in spite of its previously mentioned drawbacks.

The research group at Deakin, together with Professor Doug Macfarlane (from the School

BatTRI-Hub director Prof Maria Forsyth and Assoc Prof Patrick Howlett

of Chemistry at Monash University) and his team, have investigated the use of ionic liquids as electrolytes and their application in lithium devices. An ionic liquid is a salt that exists in a liquid phase at room temperature, and it has a high conductivity that is ideal for many real world applications. An ionic liquid is entirely made up of ions, but not all of its ions contribute to the specific charge transport required for a given device. The team has pioneered the development of new classes of ionic liquid electrolytes. The fruits of this research are implemented into devices such as batteries, solar cells and capacitors, and these new classes of ionic liquid electrolytes are now the subject of research throughout the field. New studies have shown that sodium metal ionic liquids can support an electrical potential that competes with what has been achieved using lithium metal. This work has revealed that sodium-based batteries can indeed compete with lithium-based batteries.

Professor Forsyth brings her considerable knowledge and expertise in lithium technology to the development of sodium technologies. In her work she has shown that lithium ionic liquids can meet safety standards and can operate reliably. One reason for this is that a protective solid interface can be formed when using suitable lithium ionic liquids. Recently, she has conducted lithium metal speciation studies which characterise the organisation of metal ions and anions in the electrolyte, using computational techniques such as Molecular Dynamics as well as NMR experiments. Further to this research, her group has also studied polymer electrolytes and plastic crystals as potential safe electrolytes for energy storage.

The research project

Many institutions and governments across the globe are now investing in renewable energy and embarking on the deconstruction of the fossil fuel economy. This is a global imperative with the aim of minimising anthropogenic climate change. Renewable energy plants that use solar, wind or tidal power, cannot operate in step with energy demands. This is where electrical energy storage devices come in. They will be an essential component of the grid to ensure that electricity can be provided when it is needed. Energy storage devices, batteries in particular, will then function to allow energy modulation, and increase the reliability of the future energy grid, giving renewables greater application. Lithium-based technology will not be able to meet all of the challenges faced by an emerging renewable energy system in the long term, due to the aforementioned obstacles of its economy and availability.

The main goals of Professor Forsyth and Dr Howlett's sodium-based technology project are diligent design, research and development, and necessary

A battery scientist begins long-term performance testing on a sodium coin cell

characterisation. In more detail, there are two devices that are to be developed. One is called a shuttle battery, where ions move from one electrode terminal to the other, in charge and discharge cycles. In this sense, the ions are shuttled across the battery between the electrode terminals. The other device is a hybrid capacitor which functions by releasing ions from both electrodes during the discharge process. In this case, the ions are released into the electrolyte, changing its composition as a result. The key difference between these two devices is the charge transport within the electrolyte. In the shuttle battery the sodium ion transport is the dominant process to be optimised, while in the hybrid capacitor both sodium ion and anion transport are required for device operation. Moreover, the electrochemical and physical adsorption processes at the electrodes differ and so this means that the electrolyte may need to have different chemical properties.

Controlling metal ion speciation, particularly at an electrode interface, is essential to the development of high efficiency and long term cycling stability of ionic liquid electrolytes; the precise chemistry and the component cation and anions in an ionic liquid, as well as other complexing agents that may be added to electrolyte, strongly determine the efficiency and stability of the system. In this phase of the project, ionic liquids and polymer ionic liquid gel systems are optimised for sodium ion transport.

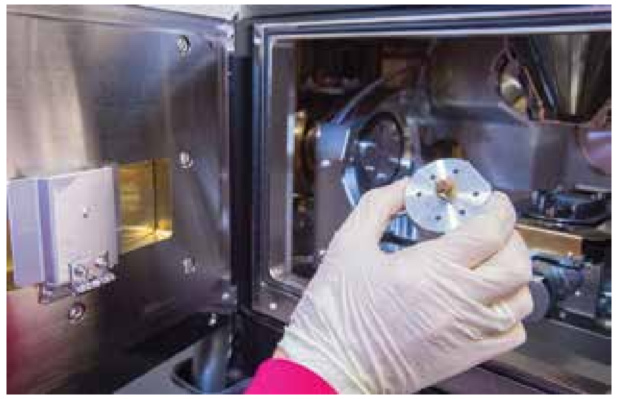
Sodium ionic liquid mixtures, where more than half of the cations in the electrolyte are in fact sodium, as opposed to typical concentrations of 5-20%, are a viable alternative that have been shown to be successful in the lithium technology sector. These mixtures offer an alternative design approach where the mixtures can be customised and optimised for ion transport, stability, electrolyte behaviour with reactive metals, viscosity, and melting point. With all these variables it is possible to finely tune an ionic liquid with the best properties for meeting the aims of the project.

The characterisation of an ionic liquid involves determining the transport dynamics and electrochemical properties of the system. The transport properties are determined by measuring the ionic conductivity at variable temperature, and measuring the viscosity and diffusion of the chemicals using advanced NMR techniques. The anions, cations and molecular solvents contain nuclei which are amenable to NMR measurements with and without an external electric field. Chemical speciation will be measured using methods that have been very useful in previous work, such as multi-nuclear NMR spectroscopy and vibrational spectroscopy. These results will be compared with measurements of the sodium chemistry, and with measurements of the ionicity – the degree to which the material exhibits ionic behaviour. Computational modelling will play a big role in development and understanding of the ion transport within the electrolytes as well as the interfacial properties of the ionic liquid at the electrode, which surely determine the electrochemical behaviour and thus ultimately the performance of the battery. Professor Forsyth's team includes a number of computational researchers who will contribute to this work.

Once a candidate electrolyte system is developed through the stages of design, development and characterisation, functional devices will be built in collaboration with Professor Michel Armand's team at the CIC Energigune from the Basque Country in Spain, for performance testing. For example, an optimised shuttle battery could be composed of a sodium metal anode with a cathode based on a sodium iron phosphate mineral ($NaFePO_4$), other layered oxide cathodes or indeed organic cathodes being developed at the CIC Energigune. Within this phase of the project, the team at the CIC will be working closely with the Deakin team to optimise the combination of electrolyte and electrode to achieve the best performing sodium battery. A cell based on the hybrid supercapacitor design would most likely have a conducting polymer or functionalised carbon cathodes newly developed by the ARC Centre of Excellence for Electromaterials Science (ACES), and a sodium anode. These devices will then undergo standard performance testing for batteries and capacitors.

Widespread benefits

This project involves a collaborative effort with institutions all over the world and will help establish Australian research on the international stage. Strong links will be forged with researchers in other fields of



Gold sputtered separator material used in fundamental studies of battery

related research, such as electrode material science and theoretical modelling. PhD students will have the opportunity to visit leading academic centres in Europe and the United States, opening up avenues for their future careers.

The team at Deakin University have also had the opportunity to apply their vast knowledge of energy storage systems to a project in collaboration with AusNet Services, a major energy infrastructure company in Victoria. This initiative involved the development of a powerful lithium battery energy bank that has been attached to the mains grid for a two-year trial period. The Deakin part of the project, led by Professor Howlett, selected the batteries and advised on aspects such as safety, service lifetime, design, experience and performance management. Just recently, the team was successful in securing an Australian Indian Strategic Research Fund grant for over $1M which will incorporate some of the outcomes from the ARC funded project, to develop prototype devices for lithium and sodium batteries. The success of this collaborative project, comprising a team of Australian and Indian based researchers, is likely to have significant impact in areas such as remote or stand-alone renewable energy installations, for example in isolated communities or rural dwellings areas of major importance to both Australia and India.

As we reduce our reliance on fossil fuels and move towards a sustainable future, efficient energy storage systems are essential. This transition is crucial in order to lessen the catastrophic effects of global climate change and environmental pollution. Supplanting fossil fuel plants in Australia with renewable energy sources alongside sodium-based energy storage technology, which would be harmoniously integrated with the electrical grid, would place Australia in a leading position in the mitigation of climate change.

Professor Forsyth and her group are poised to produce breakthrough research and bring sodium-based energy storage devices to a position where they can complement renewable energy plants in a future energy system. The synergy offered by this system can reliably meet the continuous demands of the grid and surpass our unsustainable use of fossil fuels. Sodium-based energy storage devices are therefore an essential and intelligent path forwards.

Meet the researchers

Dr Patrick Howlett
Associate Professor and Senior Research Academic
Institute for Frontier Materials
Deakin University
Burwood, Victoria, Australia

Professor Maria Forsyth
Australian Laureate Fellow and Alfred Deakin Professorial Fellow
Institute for Frontier Materials
Deakin University
Burwood, Victoria, Australia

Dr Patrick Howlett received his PhD from Monash University in Australia in 2004. Soon after, he began a postdoctoral fellowship at the same university, and went on to become a senior research fellow in 2007. In 2010, he moved to Deakin University, where he currently holds a Senior Lecturer position. Dr Howlett's research focuses on the development of new electromaterials by applying novel materials science principles, design and methodology. He has authored over 100 publications and 4 patents, which have been cited more than 4000 times.

CONTACT

E: patrick.howlett@deakin.edu.au
W: http://www.deakin.edu.au/profiles/patrick-howlett

FOCUS ON BATTERY RESEARCH

The development of safe, efficient, rechargeable batteries is key to achieving sustainable future energy supplies. This area of research will receive a major boost with the opening of a new battery technology research and innovation centre (BatTRI-Hub) at Deakin University in 2016. A major component of this centre will be the establishment of a battery prototyping facility in collaboration with CSIRO. About $1.5M has been committed to set up a facility to produce moderate sized battery pouch devices. It will also allow upscaling of materials manufacture to prepare 10-20kg batches as opposed to a few grams of electrode materials. 'The prototyping facility will be a platform for us to test our novel materials and new technologies in a more realistic format (compared to coin cells) which will be a core component for future applied research projects and future industry partnerships (both locally and internationally)', explains Professor Forsyth. 'One focus of this research will be prototyping of sodium metal batteries.' Researchers at the hub will also explore innovations in functionality, such as the development of flexible and wearable batteries, light weighting and system integration. Battri-Hub will be a centre for engagement with industry, from chemical companies through to battery manufacturers and energy providers.

Professor Maria Forsyth earned her PhD at Monash University, Australia in 1989. Since then she has held positions in the USA, UK and Australia. She is an Australian Laureate Fellow and Alfred Deakin Professorial Fellow at Deakin University. She is also Associate Director in the ARC Centre for Excellence in Electromaterials Science and Deputy Director of the Institute for Frontier Materials. Her work focuses on charge transport in electrolytes and metal-electrolyte interfaces, including ionic liquids, polymer electrolytes and plastic crystals. She leads collaborative projects in lithium and sodium battery technologies with funding from ARC. She has co-authored over 400 publications that have received over 11,000 citations in total.

CONTACT

E: maria.forsyth@deakin.edu.au
W: www.deakin.edu.au/apps/research/find-a-researcher/19894/Prof-Maria-Forsyth

KEY COLLABORATORS

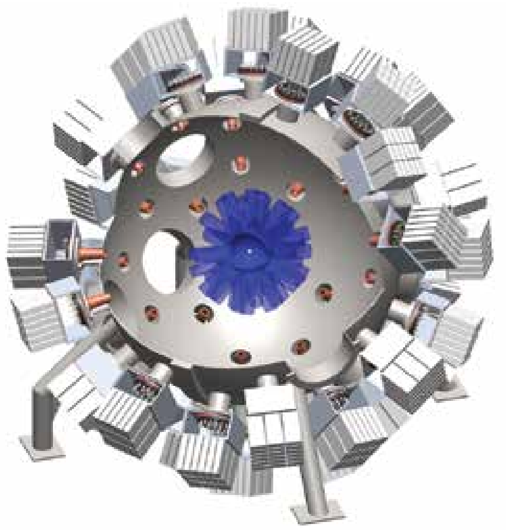
Professor Douglas MacFarlane, Monash University, Australia
Professor Michel Armand, CIC EnerGIGUNE, Spain.

FUNDERS

Australian Research Council (ARC) through the ARC Discovery Scheme

Plasma guns fire into the race for fusion

Dr. Scott Hsu is a fusion physics research scientist interested in obtaining cost efficient, clean energy for the world. His work, pursued with Dr. F. Douglas Witherspoon and others, focuses on plasma-implosion research for an alternate-fusion approach.



Dissected view showing the plasma-liner formation via 60 merging jets. Copyright HyperV Technologies Corp. 2016

What drew you towards nuclear fusion research?

I remember reading about fusion in high school and thinking that fusion energy is something that the world will eventually need. This was in the mid-1980s when achieving a burning plasma in the laboratory felt imminent. At UCLA I had the fortune to take two plasma-physics courses with Professor Francis Chen (author of the famous textbook) and work in his lab. He alerted me to a summer internship at the Princeton Plasma Physics Laboratory, where I solidified my desire to pursue a research career in fusion. I got into Princeton's graduate program in plasma physics in 1993 and, as they say, the rest is history.

How did you come to work on magneto-inertial fusion?

I always had a keen interest in alternate-fusion concepts. I went to Los Alamos to work on the solid-liner magnetized target fusion collaboration between LANL and the Air Force Research Laboratory. I quickly came to see the challenges of solid liners. The destructive nature of imploding a solid liner and its relatively slow implosion speed (demanding long-lived targets that are hard to create) contributed to a slow rate of research progress. Later I came to learn about Dr. Y. C. Francis Thio's proposed plasma-liner approach to magneto-inertial fusion (MIF), which could potentially overcome many of MIF's crippling problems. With Thio's encouragement, I organized a national workshop at Los Alamos in 2008. This led to the formation of my present research team and a winning proposal to the DOE Office of Fusion Energy Sciences to construct the Plasma Liner Experiment (PLX) and to initiate a programme researching the feasibility of forming plasma liners by merging supersonic plasma jets.

What is the project you lead and who are the principal investigators?

I lead the ARPA-E-funded PLX-α project, comprised of LANL, HyperV Technologies Corp. (F. Douglas Witherspoon), the University of Alabama in Huntsville (Jason Cassibry), the University of New Mexico (Mark Gilmore), Tech-X Corporation (Peter Stoltz), and Brookhaven National Laboratory (Roman Samulyak). They have all been involved in plasma-liner and/or plasma-jet research since the inception of the plasma guns project in 2004 or the PLX project in 2010.

The recently initiated three-year ARPA-E project will execute two experimental campaigns. The first nine-jet campaign covers an octant of our spherical chamber. The purpose is to show that a portion of a liner with sufficient quality can be formed via merging jets. If this is successful, we will conduct full spherical implosions with up to 60 jets. What we hope to learn are the scalings of uniformity and ram-pressure with convergence, the initial jet parameters, and the number of jets. These results will be used to evaluate and benchmark our computer codes, which can then be used to design full-scale plasma-jet-driven magneto-inertial fusion (PJMIF) experiments.

What promising results have you obtained?

Our prior experiments focused on characterizing the evolution of a single plasma jet propagating from the chamber wall to the merging radius and the oblique merging of two jets. From the single-jet experiments, we learned that jet propagation leads to tolerable expansion and density degradation. We measured jet parameters and profiles necessary for faithful simulations. From the two-jet-merging experiments, we learned that oblique shocks indeed form during the merging process and must be characterized in more detail in order for us to assess whether their effects are acceptable for PJMIF. Overall, our initial experiments and modeling efforts have established the scientific basis for plasma-liner formation via merging plasma jets, and encouraged us to proceed to an experimental demonstration of spherical plasma-liner formation.

How does PJMIF compare to other approaches?

One attribute of PJMIF is the low-cost MIF part of it, as compared to magnetic fusion energy (MFE) or inertial confinement fusion (ICF). We feel that lowering fusion R&D costs is essential to the timely development of fusion energy. Another is that PJMIF is a reactor-friendly embodiment of MIF that seeks to overcome the disadvantages of many other MIF approaches, such as their destructive nature and/or slow implosion velocity. The plasma guns that launch the jets will not be damaged, and their electrodes have a slow erosion rate. We can fire dozens of shots per day for faster R&D progress. In a reactor, PJMIF can in theory fire at 1 Hz, resulting in attractive power-plant economics. Another key advantage of PJMIF over MFE and ICF is the potential compatibility with flowing liquid blankets, which would serve as the high-temperature medium for breeding tritium and generating electricity, avoiding an open-ended, costly solid-materials development program.

How can PJMIF achieve that?

By using a strong magnetic field to slow down the rate of energy loss, ignition can be achieved at densities higher than MFE but lower than ICF. In this intermediate range, the combination of plasma energy and power density allows for optimum cost to generate ignited plasma (200 million USD compared to the billions to tens of billions required for mainstream fusion approaches). The plasma implodes along with a magnetic field strong enough to retard heat loss. These arguments were elegantly derived from physics first principles in a paper by retired LANL scientists Irv Lindemuth and Richard Siemon, "The fundamental parameter space of controlled thermonuclear fusion," meant for a broad audience beyond plasma-physics experts.

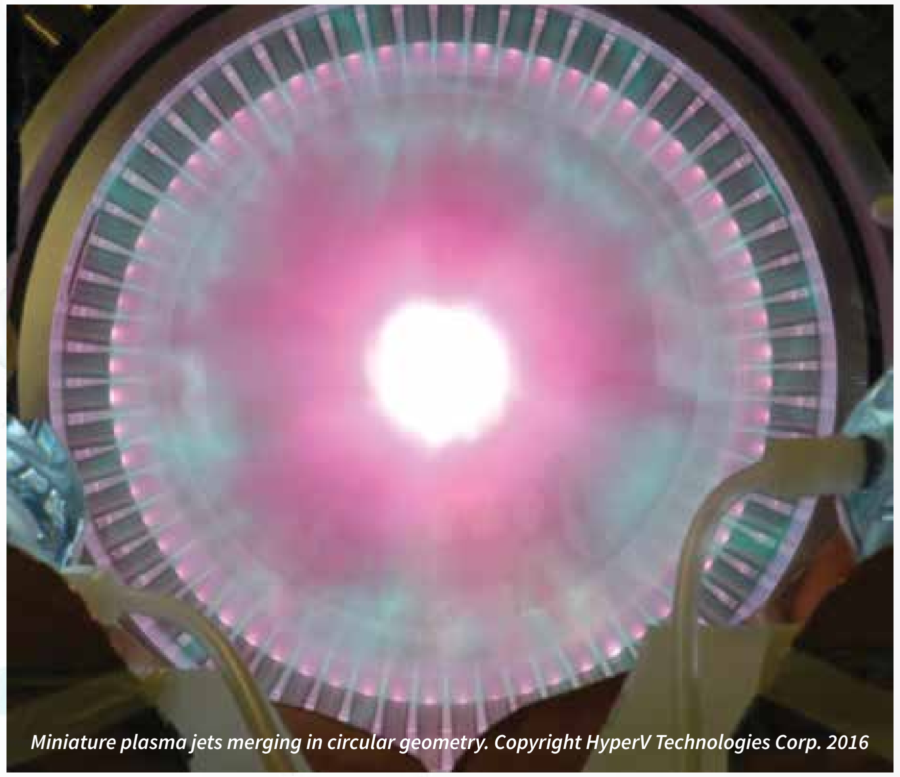
The non-destructive, standoff, and high-shot-rate nature of PJMIF is enabled by the innovative plasma guns that launch the required plasma jets for PJMIF to reach ignition conditions.

Will PJMIF reach ignition sooner than competing technologies?

If things go well, then maybe yes! However, if there is one lesson to be learned from the history of fusion research, it is that there are always unforeseeable problems, which become harder close to ignition. PJMIF enables a low-cost, high-shot-rate, rapid-learning pathway toward ignition. If ignition is achieved, PJMIF has attractive features for scaling up to a fusion power reactor. These are the main reasons we are excited by and are motivated to develop PJMIF.

Developing a cheaper, faster pathway to economical fusion power

A multi-institutional research programme is underway to develop a novel approach to fusion power in the form of plasma-jet-driven magneto-inertial fusion (PJMIF).



Miniature plasma jets merging in circular geometry. Copyright HyperV Technologies Corp. 2016

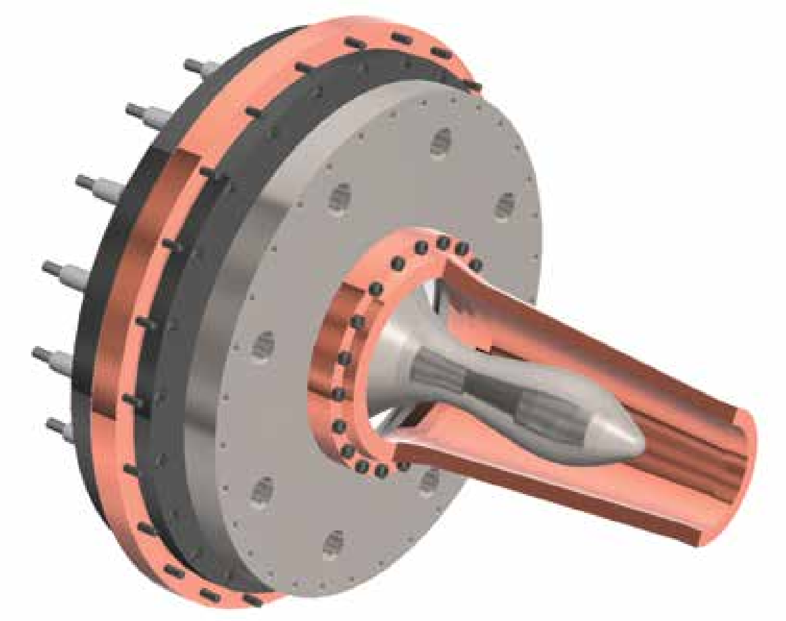
PJMIF - A NOVEL APPROACH TO FUSION

The concept of PJMIF was invented by Thio in the 1990s. It involves the use of plasma jets fired at supersonic velocities by plasma guns, which are arranged in a spherical, inward-pointing array, aimed towards a target area. The guns fire simultaneously, launching a spherical array of plasma jets that merge to create a spherically imploding plasma liner composed of a heavy element such as argon. The plasma liner compresses a magnetised deuterium-tritium (DT) plasma target to the high temperatures and pressures required for fusion reactions.

Other approaches to fusion are notably different from PJMIF in terms of reactor shapes and technologies, plasma conditions, and energy and cost requirements. ICF consists of a small, solid DT pellet that is compressed and superheated inside a cylindrical cavity by very high-power lasers positioned in a radial configuration. MFE uses torus-shaped magnetic fields to confine and heat a very large plasma, such as the tokamak.

For PJMIF, the magnetised DT plasma target is situated in the centre of a chamber, where it is compressed by the imploding liner. The liner is formed from low-temperature plasma jets travelling at supersonic speed, originating from the electromagnetic plasma guns mounted on the walls of a spherical vacuum chamber. In an orchestrated sequence of precisely timed events, the magnetised target is first created by firing only a subset of jets containing DT fuel, and in the split second that the plasma fuel comes together it is magnetised by external lasers. It is after this that the target is compressed by the trailing plasma liner. Alternatively PJMIF can be targetless, in which case the fuel is carried at the leading edge of the plasma liner itself and magnetised in a similar manner.

Plasma-liner dynamics are currently being investigated in the new PLX-α experiment, to demonstrate the viability of this approach and investigate how to scale up to larger reactors on the path to ignition – the "holy grail" of fusion research. For PJMIF this occurs when fusion reactions alone generate much more energy



View of the plasma gun. Copyright HyperV Technologies Corp. 2016

than that required to form and accelerate the plasma jets. The energy for sustained fusion would be generated solely by the fusing atomic nuclei in the plasma. Hsu also works in nuclear weapons science at LANL, affording him valuable insights into fusion ignition that most other fusion-energy researchers do not have.

APPROACH ADVANTAGES

PJMIF aims to hit an important "sweet spot" with a plasma density in the range of 10^{18}- 10^{23} cm $^{-3}$. As Hsu explains, "fusion ignition can be achieved in a pulsed system at densities much higher than those of MFE and much lower than those of ICF." To achieve ignition in this density range, a strong magnetic field is required to slow down energy loss from the plasma target. With an ideal plasma density for ignition at 10^{21} cm^{-3}, this sweet spot in "thermonuclear parameter space" affords an optimal driver-facility cost of a few hundred million U.S. dollars, in contrast to the tens of billions U.S. dollars required for MFE or ICF.

PLX, started in 2010, involved extensive computer modeling, theoretical analysis, and single- and double-jet experiments. Single-jet experiments showed that the expansion and evolving density profile of the jets is within acceptable bounds. The double-jet experiments investigated the behaviour of jet merging. The new PLX-α experiment that is now underway will first look at the behaviour of nine plasma jets. When supersonic jets merge, they form shock waves that heat and change the shape and profile of the liner. This can disrupt the uniformity of the implosion and cause liner heating, potentially leading to reduced ability of the liner to compress a magnetised target. Jet merging effects will be scrutinised in the PLX-α experiment, to pave the way for the hundreds of jets that surround the origin in a spherical arrangement in the fully realised reactor. Larger numbers of jets are favourable because they provide better implosion uniformity and lower per-gun power requirements. In future PJMIF experiments the magnetic field in the target may give a greater degree of stability against the destabilising effects of liner non-uniformities, as compared to an approach like ICF.

MIF approaches that use a solid liner can be highly destructive to experimental equipment generating the high-energy fusion processes. Destructive approaches require more maintenance and additional equipment costs, which slows research by reducing the experimental shot rate. One of the strong benefits of PJMIF is that it is non-destructive, and the electrodes used to accelerate the plasma jets have a very slow erosion rate, enabling a much higher shot rate.

FUTURE DIRECTIONS

The hydrodynamic and magneto-hydrodynamic (MHD) computational codes used to model the jet propagation and plasma-liner implosion, similar to those for describing the behaviour of stars, are not fully predictive at this point. Hsu and his team bravely tackle this challenge through carefully planned research: "The detailed nature of the plasma-liner formation and implosion processes are indeed difficult to predict via theory or computations alone, in part due to sensitivity to jet initial conditions, which are imperfectly known, and in part due to imperfect models in the codes. Our experimental R&D plan will systematically remove these uncertainties in a phased development plan". For example, this is precisely the purpose of the first nine-jet phase of the experiment. Radiation effects are to be included in radiation-MHD models which "self-consistently describe the leading-order physics of PJMIF".

The required coaxial plasma guns were also invented by Thio. They are designed and built by HyperV Technologies Corp., where experimental validation of gun performance and engineering advancements are led by Witherspoon. Today's state-of-the-art plasma guns are still in the process of being scaled up to accelerate jets with larger masses and higher densities and to achieve better control over the mass and density profiles of the jets. In terms of scalability, a large array of guns will need to function in a reproducible and reliable manner.

These new experiments will provide essential data for planning the road ahead and, in addition, inform the direction of simulations, which go hand in hand with experimental work. The best simulations of PJMIF so far are those reported by Charles Knapp and Ron Kirkpatrick. They use a one-dimensional model of the imploding plasma liner with radiation- and MHD equations. Dr. Hsu informs us that "these unoptimized 1D simulations are an indication of what is achievable, showing that energy gains of >30 may be possible." The energy gain is a parameter that is paramount for this line of research. It is defined as the ratio between the energy output and the energy input. The bigger this ratio is, the more energy the reactor produces for a given cost. Hsu and his partners hope that success in their ongoing work will lead to private investment in furthering PJMIF development for economical fusion power.

Researcher Profiles

Dr. Scott Hsu
Scientist, Physics Division
Los Alamos National Laboratory

Dr. Scott Hsu (Ph.D., Princeton University) leads the PLX-α project. He is an experimental plasma physicist with a background in magnetic fusion energy science, basic plasma physics, plasma astrophysics, and high-energy-density plasma physics. He has worked in these fields for 20+ years. His experience stretches from fundamental topics like magnetic reconnection to multiple areas of fusion research. In 2002, he was a winner of the American Physical Society's Award for Excellence in Plasma Physics Research.

CONTACT
E: scotthsu@lanl.gov
T: (505) 667-3386
W: https://www.linkedin.com/in/scotthsulanl

Dr. F. Douglas Witherspoon
President & Chief Scientist of HyperV Technologies Corp.

Dr. Doug Witherspoon is an experimental plasma physicist with 30+ years of research experience in start-up companies dedicated to applying plasma technologies to industrial, defense, space, and energy applications. He has extensive experience in pulsed-power and plasma-driven accelerators, with seven patents awarded. He leads the gun development effort at HyperV Technologies Corp., a small company dedicated to the development of commercially viable fusion-energy technologies.

CONTACT
E: witherspoon@hyperv.com
T: 703-378-4882
W: www.hyperv.com

KEY COLLABORATORS

Professor Jason Cassibry, University of Alabama in Huntsville
Dr. Samuel Brockington, HyperV Technologies Corp.
Dr. Andrew Case, HyperV Technologies Corp.
Professor Mark Gilmore, University of New Mexico
Dr. Roman Samulyak, Brookhaven National Laboratory
Dr. Peter Stoltz, Tech-X Corporation

FUNDING
ARPA-E (U. S. Department of Energy)

Capturing the forgotten source of CO2

Engineers Sofiane Zalouk and Johan Rey both work on improving the sustainability of industrial boilers. Here they describe how they have developed a carbon capture system designed specifically for intermediate emitters.

To start with, please could you describe the inspiration for this project?

The fast industrial deployment of technologies for carbon capture and storage (CCS) will be necessary if we want to make a significant impact on CO_2 emissions at the planetary scale. Nearly all the CCS pilot-scale projects in progress in various countries address the problem of high tonnage emissions, in particular from facilities like thermal power plants, iron and steel plants and cement factories. These rely upon first generation technologies that use amine scrubbing to collect CO_2 post-combustion.

The problem of emissions from sectors producing between 25,000 and 100,000 CO_2 tonnes per year, which represents a significant proportion of the total tonnage, have yet to be approached at the pilot scale. The project CO_2 EnergiCapt aims to fill this gap by developing the first pilot CCS project dedicated to heat production units for district heating, as an initial target.

Why is carbon capture technology going to be so important in the future?

Carbon dioxide capture could play an important role in reducing greenhouse gas emissions. The greenhouse gas making the largest contribution from human activities is carbon dioxide. It is released by burning fossil fuels; for example from combustion and by certain industrial and resource extraction processes. Emissions of CO_2 due to fossil fuel combustion are virtually certain to be the dominant influence on the trends in atmospheric CO_2 concentration during the 21st century.

Why has no one attempted to solve carbon capture for mid-range emitters before?

The emitters that generate large centralised amounts of CO_2 are today the priority, in particular electric power plants. For example, the primary source of greenhouse gas emissions in the United States is electricity production, which was responsible for 31% of greenhouse gas emissions in 2013. Approximately 67% of our electricity comes from burning fossil fuels, mostly coal and natural gas. But solutions also need to be found to address the intermediate emitters, which together account for a substantial amount. These emitters represented 21% of greenhouse gas emissions in 2013.

Have the results from your demonstration project been promising?

The results are actually very promising. Firstly, we reached a CO_2 capture efficiency of 85% and this could easily be raised to 90%, because our system features independent gas and solvent streams. Increasing the solvent stream used to capture the CO_2 or decreasing the gas stream from the source of emissions is quiet easy and can both drive efficiency up to 90% or more as long as you have enough solvent and a powerful enough pump.

The real technological bottleneck mostly concerns the liquid to gas ratio, the membrane's behaviour when interacting with the flue gas, the membrane's thermal behaviour and the steadiness of the capture. Since the start of the project, many interesting and promising results have been gathered on these topics.

What have been the main technical challenges you have had to overcome while developing the solution?

The main technical challenge was the design of the absorption unit since the feasibility of absorption from real flue gas using a hollow fibre membrane contactor was still unproven at the beginning of the project. Then, the choice of the membrane-solvent pairing and the design and implementation of the pilot were obviously also some of the most critical parts.

What is the next step for the project?

The project will end at the end of the year so there are several next steps intended after that. First, next year we will start a Power-To-Gas project called JUPITER 1000 in France for a period of five years. In this project, Leroux & Lotz Technologies is responsible for building a CCS unit using the EnergiCapt process to collect CO_2 and convert it into methane via a methanation reaction.

At the same time, we are very interested in testing our technology on different flue gases like those from coal boilers or biomass boilers, as well as those from different industries like the cement industry or power plants. We are looking for partners to do so, but we are also likely to test our process on our own boilers since we are boiler manufacturer.

The reduced footprint of our membrane technology makes our process very suitable for industries with limited space, for instance oil platforms. We are therefore very interested in applying our process in different area like natural gas extraction, de-acidification and enhanced oil recovery.

Novel approach to CO2 capture slashes footprint and energy costs

Traditional methods of carbon capture are both bulky and energy intensive, which limits its adoption by medium scale emitters. Now Leroux & Lotz Technologies have developed a system that uses a new capture method and improved energy integration to tackle both problems at once.

A PRESSING PROBLEM

There is an overwhelming consensus among scientists that CO_2 released due to human activity is directly causing the most rapid increase in global temperatures in history. But despite this stark warning, emission levels continue to rise across the globe.

While carbon-free alternatives exist for power generation, fuelling vehicles and heating our homes, they have yet to reach a point where they are cost competitive with fossil fuels. As a result, convincing politicians and business leaders to abandon the energy source our industrialised society was built on is likely to be a long and bumpy road.

But while eliminating CO_2 emissions from fossil fuels may be too ambitious a goal in the medium term, carbon capture and storage (CCS) technologies have in recent years emerged as a potential stop gap. These systems are designed to remove CO_2 from the exhaust flue gasses produced by emitters before storing it deep underground.

The oil and gas industry has been using the process to store waste CO_2 separated from extracted natural gas for years and there are several pilot projects to remove CO_2 from industrial emissions currently under development. These projects are almost exclusively concerned with the largest emitters of CO_2 such as fossil fuel power plants, the steel industry and cement factories.

But according to the US Energy Information Administration, intermediate emitters producing between 25,000 and 100,000 tonnes of CO_2 per year are responsible for up to 21% of greenhouse gas emissions. This is what prompted French industrial boiler company Leroux & Lotz Technologies (L&LT) to launch their "CO_2 EnergiCapt" project in 2011. Funded at 30% by the French National Research Agency (ANR - France) with the remainder coming from L&LT, the scheme is designed to address the need for carbon capture technology tailored to smaller CO_2 emitters.

photo credits: Leroux & Lotz Technologies

TAILORING THE SOLUTION

Most current CCS technology is both large and energy hungry. While this is less of a problem for large facilities like power stations, for smaller emitters such as district heating plants or the agri-food industry, these limitations make the use of CCS unfeasible. As a result, R&D research manager Sofiane Zalouk and R&D engineer Johan Rey came up with an entirely novel system that helps to address both problems.

Traditional CCS solutions rely on absorption columns, where solvents that absorb the CO_2 are fed in at the top and exhaust gasses are fed in at the bottom. CO_2 is removed from the fumes by the solvent, which becomes saturated with CO2 and collects at the bottom, while the treated exhaust now low in CO_2 escapes from the top.

These systems have a very large footprint though, so instead Zalouk and Rey decided to use hollow fibre membranes – a form of semi-permeable barrier used to separate gasses and liquids – to create much more compact "contactors". The membranes were fashioned into cylindrical tubes, with the solvent running through the centre of the tube while the exhaust gasses pass over its exterior.

"This brings many advantages," says Rey. "Firstly it decreases the footprint as the contactors offer very high specific surface, which makes the unit a lot smaller than an absorption column. Secondly there is no contact between the flue gas and the solvent, which both decreases pollution of the flue gas and solvent degradation. It also increases the system flexibility as the streams of flue gas and solvent are independent."

In 2013 a demonstrator was set up at a district heating plant in Paris run by CPCU, to test the design on the flue gasses emitted by a 140 MWth gas boiler. The first step in the process involved a flue gas condenser that cooled down the fumes to remove moisture to avoid condensation in the contactor that can reduce capture efficiency, as well as recover condensation energy. After being condensed the gasses then passed to the contactor, which contained a solvent consisting of 70% water and 30% ethanolamine, a chemical commonly used to absorb CO_2. After this the solvent passed to a desorption column where the CO_2 was stripped from the solvent.

PROMISING RESULTS

While the small-scale prototype only treated 0.2% of the gas emitted, tests using a gas analyser showed that the system was capable of a capture efficiency of 90% - comparable to traditional CCS methods. According to Zalouk, the tests also gave the engineers valuable data on the correct ratio of solvent to gas, the membrane's interaction with real flue gas and how the contactors respond to different temperatures.

"The project has also given us invaluable experience in designing and operating the demonstrator, which is very important for us since our trade is to design, integrate and set up," he adds. "By the end of the year, we will also get data on the energy cost of the process and its impact on the plants, and will be able to scale up all our results."

As well as introducing a novel method for capturing –-, the engineers also worked on improving the energy integration of the process to address the other major limitation of CCS technology – energy costs. This involves making the most efficient use of all energy sources available in the process or on site.

Rey says the design of energy integration measures is specific for each case and depends on heat sinks available on site. The aim is to build a kind of synergy between the factory and the capture unit while limiting the impact on the existing process, for instance on the boiler's efficiency. But with their demonstrator the engineers were able to use the flue gas condenser to preheat the solvent before the desorption unit, which reduced the energy required to desorb the CO_2. They also used the sites cold water network instead of a refrigeration unit to cool the solvent before the absorption unit, which is operating at low temperature (20-30°C), and to cool at the desorption unit outlet the CO_2 was stripped from the solvent in order to condensate steam and maximize the CO_2 purity until 98%w.

SCALABLE AND VERSATILE

While the project run by L&LT does not address the question of what to do with the CO_2 once it has been captured, the company has since 2015 become involved in a French project called Jupiter 1000, which will combine captured CO_2 and hydrogen from water to create methane gas. L&LT will use its EnergiCapt process to provide the CO_2 required for the process. "Methanation is a very interesting way to use and convert CO_2 since the CH4 produced is an energy source which can be directly injected in the natural gas network, or easily kept as stock." says Rey. "manifold ways exist for CO_2 from capture technologies, for example: oil recovery, refrigerant, Bio-transformation into fuel.." complements Zalouk.

The demonstrator project finishes at the end of 2015, but the researchers are confident they will be able to find further test beds for their solution. "This technology is mainly modular thanks to the membrane contactor, which mean scaling up or scaling down is very easy," says Zalouk. "The fact that it can be retrofitted is also very important because the technology is then suitable for all the industries and CO_2 emitters we talk about.

"With the high compactness of the technology thanks to the membrane contactors, the ability to retrofit makes the installation and the integration of the unit as simple as possible, without requiring any modifications on the boiler or the process. The capture unit can be considered as a kind of "black box" that can be plugged on to any flue gas outlet as a filter."

Lastly, a special acknowledgement. This work has been supported by French Research National Agency (ANR) through Efficacité énergétique et réduction des émissions de CO_2 dans les systèmes industriels program (project CO_2-EnergiCapt n°ANR-10-EESI-03).

Researcher Profile

Sofiane Zalouk is a process engineer and R&D Manager of the Industry Business Unit of Leroux & Lotz Technologies. He runs projects related to energy optimisation and more environmentally friendly processes, like CCS. In 2005 he received his masters degree in industrial engineering from Paul Cezanne Marseille University and in 2009 he received his PhD from Aix-Marseille Provence University

CONTACT
E: sofiane.zalouk@lerouxlotz.com
P:+33 2 40 95 96 97
W: http://www.lerouxlotz.com/

Johan Rey is a process engineer and R&D Engineer in the Industry Business Unit of Leroux & Lotz Technologies. He primarily works on CO2 capture and conversion by power to gas. In 2011he received his a M.Sc degree in Process and Electrical Engineering at Université Claude Bernard Lyon and in 2013 he received his M.Eng in Process Engineering at UTC – Compiegne whilst undertaking an internship at Leroux & Lotz Technologies.

CONTACT
E: johan.rey@lerouxlotz.com
P:+33 6 16 18 36 41
W: http://www.lerouxlotz.com/

FUNDING
Leroux & Lotz Technologies
French National Research Agency (Agence Nationale de la recherché-ANR)

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