PRACE DIGEST 2021

Changing the world

PRACE Digest 2021
www.prace-ri.eu

Editor-in-Chief
Marjolein Oorsprong – PRACE Head of Communications Office

Article Editor
Harry O'Neill, Insight Media Group

Communications Manager
Sam Davis, Insight Media Group

Graphic Design
William Davis, Insight Media Group

Published by Insight Media Group, Bristol, UK

The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class high-performance computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by 5 PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 823767.

Published: November 2021
ISBN: 9789082942293

Foreword

Scientific discovery continues to prosper

Science impacts upon almost every level of the human experience. In good times, it helps make our most fanciful ambitions and ideas a reality. In harder times, we lean upon it to help us and comfort us. But although sometimes the limelight may shine harder on one side of this coin, research on both sides continues.

Since the beginning of 2020, the world has been dominated by the impacts of COVID-19. Last year, this publication reflected that, as PRACE prioritised research into reducing the impacts of this devastating pandemic. This year, however, we want to highlight research that has continued to progress in other domains of research beyond this.

Human curiosity about that which exists beyond our Earth dates back to prehistory, with a 32 500-year-old carving on a mammoth tusk found in Germany thought to be the first ever star chart. Technology has moved on since then, but our thirst for knowledge about the universe remains undiminished. Find out more about the latest research into the sun (page 28), neutron stars (page 18 and 24), and the first billion years after the Big Bang (page 6) in this publication.

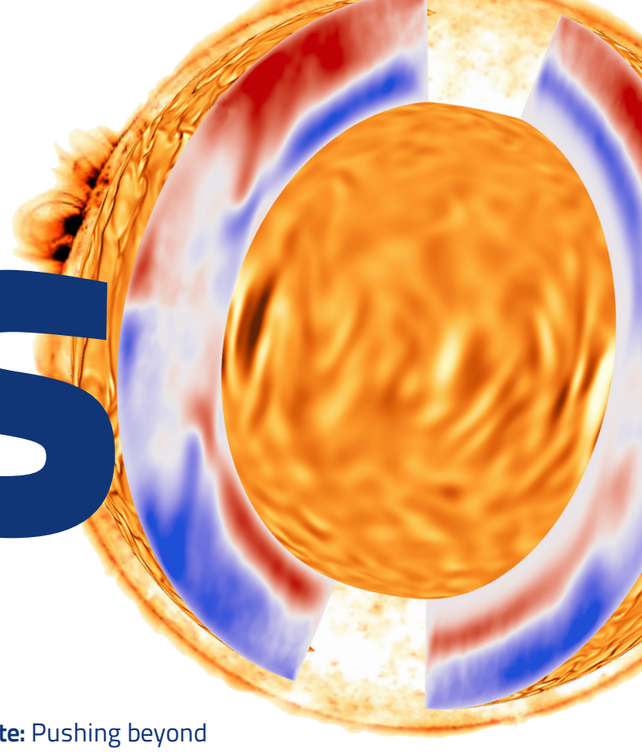
One of the hallmarks of civilisations throughout the ages has been the development of new materials that facilitate ever more powerful technologies. The field of materials science is one in which high-performance computing is playing an ever more significant role each year.

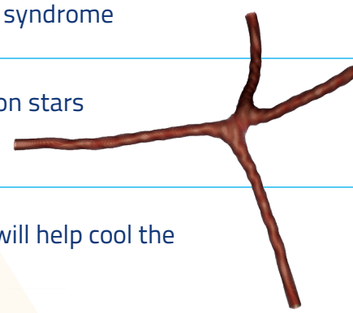
This year we bring you research on perovskites that exhibit negative thermal expansion (page 30), a quantum exploration of the latest solar technologies (page 14), and a study on the aerodynamics of ribbed surfaces based on micro-scale patterns found on bird feathers and shark skin (page 8).

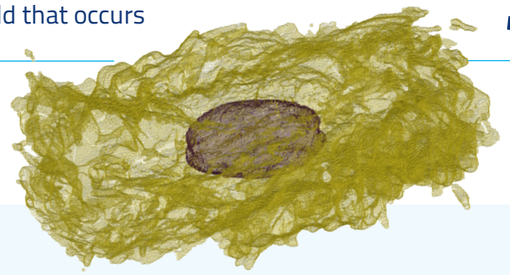
High-performance computing continues to make inroads into new domains of research with every year that passes, and we hope you enjoy the huge breadth of scientific knowledge contained within the PRACE Digest 2021. As the world starts to see a glimmer of light at the end of the COVID-19 tunnel, we hope you can take comfort in the fact that scientific curiosity remains alive and kicking in every aspect of our lives.

Serge Bogaerts
Managing Director of PRACE aisbl

Contents







Deciphering redshifted 21-cm signals

The cosmic dawn

With the development of the Square Kilometre Array (SKA) telescope, scientists are about to receive huge amounts of data that will shed light on the first billion years of the universe after the Big Bang. **Andrei Mesinger** of Scuola Normale Superiore in Italy has been involved in a PRACE project that will help decipher this data that contains a wealth of new knowledge in the field of astrophysical cosmology

The genesis of our universe has long been a source of fascination for astrophysicists, but the technological challenges of gathering data about these early stages after the Big Bang has meant that much of it remains a mystery. This is all set to change, however, with the construction of the Square Kilometre Array (SKA) telescope. Professor Andrei Mesinger of Scuola Normale Superiore, Italy, has been preparing for this by developing methods for deciphering the incoming avalanche of data.

Professor Andrei Mesinger

"My aim as a scientist is to try and understand the early universe, the first billion years after the Big Bang," says Mesinger. "In this time the universe expanded and cooled, and the first structures that would eventually become stars and galaxies took shape. After these first galaxies formed, the light from them spread out and eventually percolated all of space. I am investigating these cosmic milestones, known as the cosmic dawn and reionisation, by developing theoretical models for how the first galaxies and the intergalactic medium – the web structures in between galaxies – evolve. But to confirm whether these models are accurate, we need to compare them to real data."

Fortunately for Mesinger, a wealth of such data is set to become available in the form of radio maps that will be produced by the Square Kilometre Array (SKA) telescope. The signal being detected is known as the redshifted 21-cm signal. Corresponding to the spin-flip transition of neutral hydrogen, which makes up the majority of the universe, the 21-cm line can provide information about the temperature and ionization state of cosmic gas. The data being collected by SKA is therefore set to transform astrophysical cosmology, bringing a historically data-starved field into the era of Big Data.

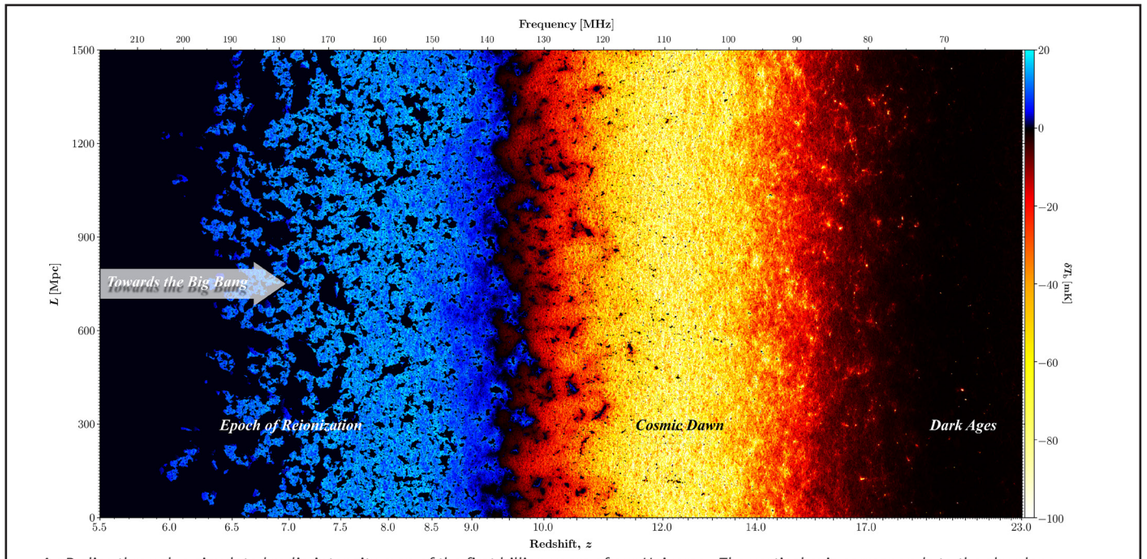
More information
https://arxiv.org/abs/2107.00018

HPC Resources awarded by PRACE
This project was awarded 20 000 000 core hours on Piz Daint hosted by CSCS, Switzerland.

Crucially, with the development of new interferometers like SKA, these 21-cm signal radio maps will allow researchers to map out the first billion years of the universe, enabling them to learn about the properties of the unseen first generations of galaxies. Data from SKA is expected to start arriving around ten years from now, but preparatory work has already begun so that researchers can hit the ground running when the telescope becomes functional. Mesinger has recently been leading a PRACE project called "AIfor21CM – Artificial Intelligence for 21-cm Cosmology", which was awarded 20 000 000 core hours on Piz Daint hosted by CSCS, Switzerland, and aimed to optimise the analysis of the upcoming 21-cm images.

Deciphering these signals presents a difficult challenge. "We know that the radiation from galaxies drives the patterns in these signals, and if we assume some galaxy model, we can predict what the signal should look like," says Mesinger. "But the question then is: how can we statistically compare these predictions to actual observations, in order to see which galaxy model is correct?"

The 21-cm signal is highly non-Gaussian, and so the common approach of compressing the images into a power spectrum (PS) summary statistic wastes potentially valuable information. Therefore, to extract as much information as possible from the signal, Mesinger and his team have made use of convolutional neural networks (CNNs). CNNs are especially useful for this purpose because they can adaptively select the optimal summary statistic that maximises their ability to recover astrophysics.



A 2D slice through a simulated radio intensity map of the first billion years of our Universe. The vertical axis corresponds to the sky plane (spanning an angular size of roughly 15 Moon diameters), while the horizontal axis corresponds to lookback time (further towards the right corresponds to earlier times/further distances). Radiation from the first galaxies in our Universe imprints the large-scale patterns seen in this map. If we can "decipher" these complex patterns, we can learn the unknown properties of the unseen first galaxies.

"Our method involves using training sets where we know the right answer, which we use to teach the CNN to find the right answer," explains Mesinger. "This is where the PRACE project came in. Our original work was severely limited by computational resources; network tuning was done "by hand" using only a few configurations, since each training of the CNN took days on our local CPU cluster. However, this PRACE project has allowed us to optimise the performance of our CNNs by using the efficiency of GPU clusters. We were able to introduce recurrent layers to our CNNs, which although very expensive to train, can efficiently follow the evolution of the maps along cosmic time."

Moreover, since the parameter space of adjustable hyper-parameters (governing the network architecture) is enormous, running an automatic optimisation requires hundreds of thousands of CNN trainings. This can only be done on a Tier-0 GPU cluster like PizDaint. The end goal of this research is an optimised artificial neural network trained to infer the properties of the unseen first galaxies from realistic 21-cm images of reionization and the cosmic dawn. Having such a tool will enable researchers to understand the data gathered by SKA, thus maximising Europe's significant investment in the experiment.

The data being collected by SKA is set to transform astrophysical cosmology, bringing a historically data-starved field into the era of Big Data.

The project is now completed, but a numbe of obvious extensions to the work remain, as Mesinger explains: "Now that the networks have been trained, the next step is to do this in a fully Bayesian way. Right now, the networks give us a best guess, but we do not have a great idea of the uncertainty of this best guess. Our next move would therefore be to combine the predictions from neural networks with a Bayesian inference framework."

Mesinger and his team ran into several technical problems during the PRACE allocation due to the demanding nature of their calculations, both in terms of processing power and RAM. "The staff at the centre were very helpful the whole way through, assisting us in restructuring how the data was loaded in and out of memory, and writing a bottleneck-free I/O pipeline. This was crucial for our huge data demands," adds David Prelogovic, a PhD student of Mesinger and lead author on the resulting scientific paper. "Having them there helped us to make this project a success, and we hope this work will prove to be useful when SKA finally starts to deliver data," concludes Mesinger.

Convergent-divergent riblets

Bio-inspired surfaces for reducing flow separation

Inspired by micro-scale surface patterns found on bird feathers and shark skin, a research team from the STFC Daresbury Laboratory and the University of Manchester led by **Dr Jian Fang,** has been exploring the use of structures known as convergent-divergent riblets for controlling aerodynamic flow, which could help to improve efficiency and reduce energy use in several engineering applications.

When air passes over a wing, the strong pressure gradient can cause the flow to become messy and separate from the surface. By attaching fin-like structures called vortex generators close to the leading edge of the wing, it is possible to help the flow resist this surface separation and remain well-attached to the wing.

Dr Jian Fang

Although widely used today in various aerodynamic applications, one issue with vortex generators is their relatively large size, which can disturb the entire flow field if not used properly. To get around this limitation, researchers have been turning to nature for help, as Jian Fang of the STFC Daresbury Laboratory explains: “Sharks and birds are both well adapted to moving efficiently through fluid, be it water or air. If you examine shark skin or bird feathers under a microscope, they both share a common feature: small directional grooves invisible to the naked eye that are used to control the flow of fluid over the surface.”

Inspired by these bio-designed surfaces, Fang and his colleagues have set about exploring the possibility of using similar patterns in engineering. Naming their own version of these structures convergent-divergent riblets (CDRs), they have been using resources awarded by PRACE to confirm how CDRs are able to produce vortices, and to carry out a parametric study to explore the effects of various characteristics of the structures.

The project used a high-order finite difference flow solver developed by Fang called the ASTR code, which is a powerful tool for exploring the details of a given flow. In this study, the researchers carried out direct numerical simulations of a channel flow with CDRs implemented on the top and bottom walls, and fully resolved the turbulence down to the smallest scales to acquire every detail of the flow fields and see which parameters had the biggest effect on controlling the flow.

More information
https://scholar.google.com/citations?user=CcZ2Oz0AAAAJ&hl=EN

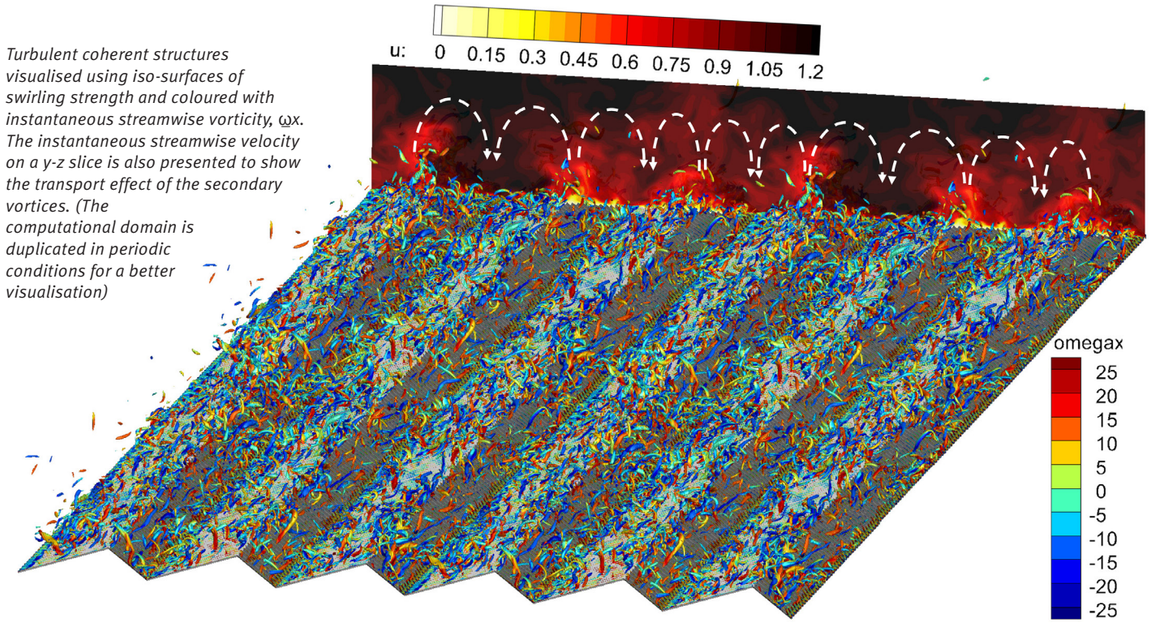
HPC Resources awarded by PRACE

This project was awarded 60 000 000 core hours on Hawk hosted by GCS at HLRS, Germany.

The project began by looking at the influence of the spacing between riblets. “In the flow field we could see that CDRs enhance momentum exchange and provide resistance to flow separation by generating what we call large-scale streamwise vortices,” says Fang. “As we increased the spaces between the riblets, the vortices became stronger, and through our simulations we were able to find the point at which the spacing produced the largest effect.”

Following this, the effects of the riblets on turbulence were explored. The CDRs, as expected, increased the levels of turbulence due to the enhanced momentum exchange that they produce. This stronger turbulence increased the levels of drag due to the increased friction against the surfaces of the channel. “What we found here is there is a trade-off between reducing flow separation at the cost of increased drag,” explains Fang. “However, we believe it might be possible to achieve reductions in both, which will be the subject of further studies.”

The next part of the study looked at the effects of the width of the converging and diverging strips. Narrower strips produced smaller vortices, while wider strips produced larger vortices. The ability to tune the size of the vortices by changing this parameter is an excellent characteristic of CDRs, as it provides the potential for engineers to refine the CDRs for specific applications, which is not possible with standard vortex generators.



Turbulent coherent structures visualised using iso-surfaces of swirling strength and coloured with instantaneous streamwise vorticity, ωx. The instantaneous streamwise velocity on a y-z slice is also presented to show the transport effect of the secondary vortices. (The computational domain is duplicated in periodic conditions for a better visualisation)

Finally, the researchers studied the influence of the configuration of the riblets on performance. “In the standard configuration, we placed riblets all the way across the surface. Then, we trialled several different patterns, for instance gradually reducing the height of riblets towards the convergence lines,” says Fang. “We saw that the configuration of the secondary vortices was correlated to the configurations of these riblets.”

All of the simulations have now been completed, and Fang’s team is still analysing the wealth of data they have produced. What has been shown for certain is that the CDRs are able to generate large-scale vortices that can reach the entire height of the channel, and that the scale and strength of these vortices can be tuned by adjusting different parameters. In an ongoing study, the team are examining the effects of CDRs in Mach 2.9 supersonic flows, in which shockwaves can induce flow separation, and preliminary simulations have shown some promising results.

As we increased the spaces between the riblets, the vortices became stronger, and through our simulations we were able to find the point at which the spacing produced the largest effect.

The resources provided by PRACE to Fang’s team have been fundamental to the research, as his colleague Charles Moulinec explains. “Before beginning this project, we were granted resources from PRACE to test out the code’s performance at scale on up to 100 000 cores. The results of this helped to shape the proposal for the project, as it allowed us to know with confidence that the code could run in an optimal way at this scale.”

Fang himself is also full of praise for what these computing resources and PRACE’s support has helped them achieve: “Without PRACE, this work could not be done. Here in the UK we have access to some Tier-1 and Tier-2 machines, but the high complexity of the meshes we used and the mathematical transformations we used to build them meant that Tier-0 resources were a must.

“Much of this work was done during lockdowns in the UK caused by the COVID-19 pandemic, and even then we were able to easily access the computing resources from our homes. PRACE also provided us with excellent opportunities for training in which we were able to optimise and tune the ASTR code. From there, we were inspired to reengineer the code to improve the IO performance, and this new version of the code will soon be released.”

Molecular dynamics simulations

Understanding the biomolecular nanomachines in our cells

Dr Mert Gur of Istanbul Technical University is studying the tiny cellular engines known as dyneins, motor proteins that convert chemical energy to drive movement in our cells. By modelling their thermodynamic cycles, he hopes to provide crucial information that will improve our understanding of diseases like Alzheimer's and cancer, as well as opening up new possibilities in nanotechnology

If you've ever found yourself getting frustrated at your train not turning up on time, you might be annoyed to hear that the inside of your own cells are probably better connected than your local town or city. Microscopic 'railway' systems made up of tiny tracks called microtubules – each of which are just 25 nanometres wide – connect all of the important destinations within our cells. Cargo can be transported along these tracks to ensure cellular functions and homeostasis are maintained. But if microtubules are the cellular tracks, what are the cellular trains?

Associate professor Dr Mert Gur

The answer is motor proteins, tiny cellular engines that convert chemical energy stored in ATP to drive movement. With a background in mechanical engineering, Dr Mert Gur of Istanbul Technical University found himself drawn to working out how these cellular dynamos work. "Motor proteins are fascinating to me because they function exactly like a car engine," he says. "Much like a car, they take a fuel – ATP – and break bonds in it to release chemical energy. This is then converted into mechanical energy, which can be used to transport cargo, move flagella, or prepare the cell for mitosis."

To understand how these biomolecular nanomachines work, it is useful to first imagine how more familiar machines work. "When we look at a device such as a car engine, we see that it operates on a thermodynamic cycle," says Gur. "This means that it starts at one point, does whatever it needs to do, comes back to the same point, then repeats. Revolutions per minute of a car engine is in fact therefore a measure of the number of thermodynamic cycles happening per minute. Proteins are the same – they start at one point, do their function, come back, then do it again and again."

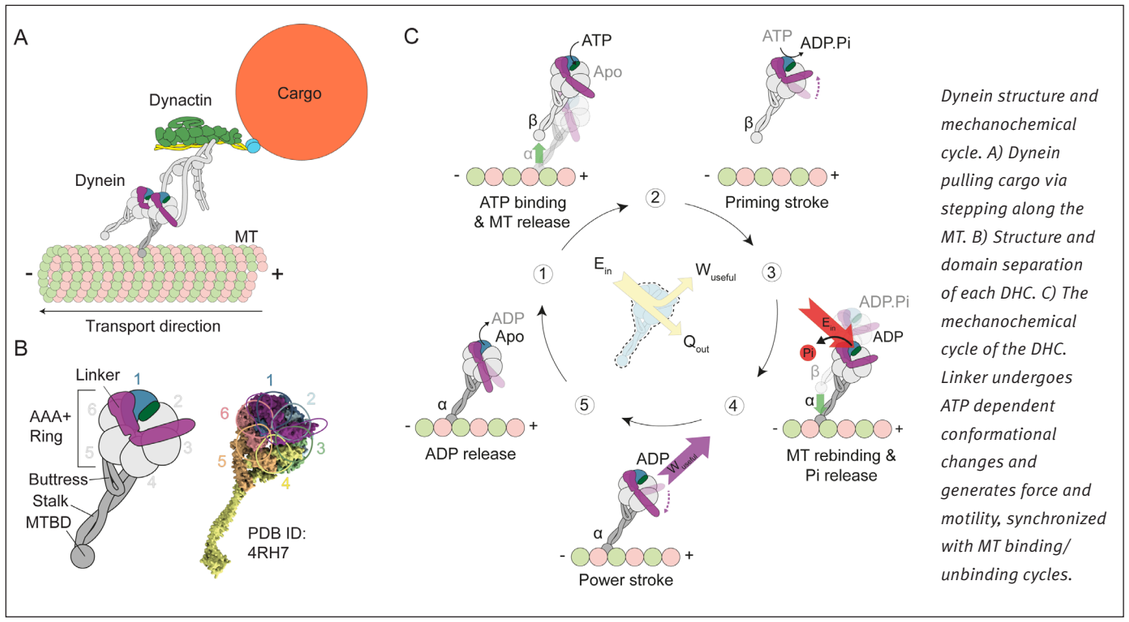
More information
https://gurlab.itu.edu.tr/en/

HPC Resources awarded by PRACE
This project was awarded 48 400 000 core hours on Marconi100, hosted by CINECA, Italy.

Gur has been leading a PRACE project, which is performed in collaboration with Ahmet Yıldız of UC Berkeley (USA) and Andrew Carter of Medical Research Council (UK), with the aim of modelling the thermodynamic cycles of a family of motor proteins called dyneins. Interest in these molecules lies not only in their role in disease – problems with dyneins are linked to both developmental and neurological disorders– but also their potential for the field of nanotechnology, which as yet does not contain within its arsenal molecules that are capable of functioning as engines, converting chemical energy into mechanical motion.

To understand exactly how dyneins work, Gur uses molecular dynamics simulations to fill in the gaps in experimental knowledge. "When looking at how a protein functions, experiments can only get you so far," he explains. "They can provide you with an atomic structure of the protein, but what you actually get is the protein frozen at one point along the thermodynamic cycle.

"It is possible to take a number of these snapshots to deduce how the protein might work, but it is not possible to experimentally capture how the protein gets from one point to another at atomistic detail. What molecular dynamic simulations do is to provide the link that shows the dynamic transition of a protein from one structural state to another."
The best way to describe the way dyneins move along microtubules is "walking". Two monomer legs connected by a linker domain move one after the other, attaching and reattaching further along the microtubule to make forward progress. The movement is powered by the ATP hydrolysis cycle. ATP binding to the dynein causes its release from the microtubule and ATP hydrolysis triggers a conformational change in the linker domain (called a priming stroke), which pushes dynein in the forward direction. After this, dynein rebinds to the microtubule, and releases the inorganic phosphate. Subsequently, the linker moves back to its original position, and this generates the force-generating power stroke that enables dynein to pull the cargo in the forward direction.



Dynein structure and mechanochemical cycle. A) Dynein pulling cargo via stepping along the MT. B) Structure and domain separation of each DHC. C) The mechanochemical cycle of the DHC. Linker undergoes ATP dependent conformational changes and generates force and motility, synchronized with MT binding/ unbinding cycles.

Gur and his colleagues have successfully modelled the priming stroke of the linker, showing in detail the mechanism and energetics of this process. They have also modelled how dynein interacts with specific residues on tubulin and stably binds to microtubules. More recently, Gur has studied how microtubule-associated proteins (MAPs) regulate microtubule binding of dyneins. "Overall, we have been able to explore some of the most critical aspects of the thermodynamic cycle of dynein in this project," says Gur. "This is a significant contribution to the field as dynein's mechanochemical cycle has not been simulated at atomistic detail before."

> *This is a significant contribution to the field as dynein's mechano-chemical cycle has not been simulated at atomistic detail before.*

Gur is enthusiastic in describing the transformational effect of having access to Tier-0 resources to his research. "As a scientist working in a computational field, it's like a dream having this amount of power at your fingertips," he says. "Usually, you are in a position where the computational power available to you lags far behind the speed of your thoughts – it will take months to confirm just one idea through a simulation. With the resources provided by PRACE, this time was cut to a matter of days.

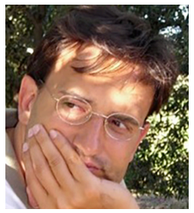
"As well as this, this project has opened up a number of new collaborations with other labs working on dyneins. There are not many people working in this particular field, as the system size of the dynein molecule solvated in water – around one million atoms – has meant that up until now, simulating it has been out of reach in terms of the limits of computational power today. Thanks to PRACE, we have carried out some of the first molecular dynamics simulations of these proteins, so I am grateful for this opportunity – it has been a great experience."

Anomalous magnetic moment of muons

Exploring the Standard Model to discover the physics beyond

Professor Leonardo Giusti of the University of Milano - Bicocca has been using supercomputers to explore the Standard Model and, in particular, developing a new algorithmic invention to measure the specific properties of one of its fundamental particles - the muon. The work concentrates on the discrepancy between the theoretical prediction of the anomalous magnetic moment of muons and its experimental value, and the idea that there may be new physics at play which is causing this anomaly

The discovery of the Higgs boson at the Large Hadron Collider in 2012 represented the last missing piece of the Standard Model, the crowning achievement of modern particle physics. Today it explains the results of experiments conducted in laboratories on a huge variety of processes. However, evidence from astrophysics and theoretical arguments suggest that the Standard Model may in fact be an effective low energy description of a more fundamental theory.



Professor Leonardo Giusti

Professor Leonardo Giusti of the University of Milano - Bicocca is a theoretical physicist who uses high performance computing to try to explore the Standard Model and look for hints of the physics that may lie beyond it. In particular, he has been working on algorithmic developments for measuring specific properties of one of the fundamental particles of the Standard Model – the muon.

Muons, along with electrons and tauons, make up a category of particles known as leptons. “Muons are essentially very similar to electrons, with the same quantum number and fundamental properties, but are around 207 times heavier,” says Giusti. Just like electrons, muons have a property called the magnetic moment, which dictates how the muon interacts with magnetic fields. In 1928, predictions for values of this property for electrons were made by Paul Dirac by combining special relativity and quantum mechanics.

More information

https://en.unimib.it/leonardo-giusti

https://virgilio.mib.infn.it/~lgiusti/lgiusti.html

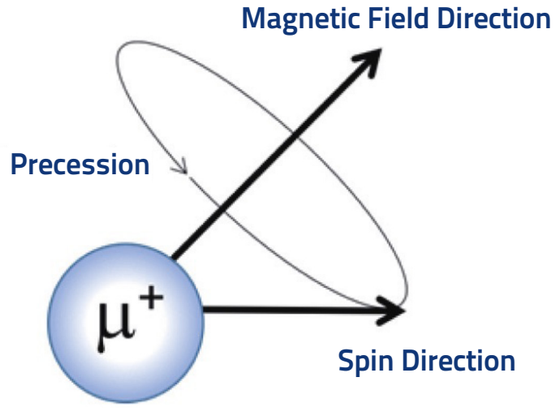
HPC Resources awarded by PRACE

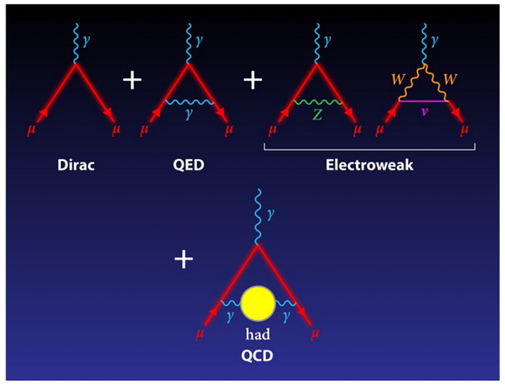
This project was awarded 40 000 000 core hours on JUWELS, hosted by GCS at FZJ, Germany.

However, it is now known that the magnetic moment of a particle such as a muon is also affected by the existence of other fundamental particles. This causes a deviation from Dirac’s prediction which is known as the anomalous magnetic moment. In the 1950s, this anomalous portion was first computed and also validated through experiments for electrons and muons. This in turn validated the theory of quantum electrodynamics and allowed for the Standard Model to be built based on what is known as quantum field theory.

The most precise measurements of the anomalous magnetic moment of the muon today have a precision of 0.35 parts per million, achieved by the E821 experiment at the Brookhaven National Laboratory and the E989 experiment at Fermilab. “The most recent number from Fermilab was released in April 2021, and it was similar enough to the figure released from Brookhaven for experimentalists to say with good certainty that it could be trusted,” says Giusti.

Interestingly, theoretical predictions of the anomalous magnetic moment based on other observables differ from these experiments by more than four standard deviations. This discrepancy has given rise to the idea among high energy physicists that there may be new physics at play, as yet not understood, which is causing the discrepancy between the theoretical prediction and the experimental value. So where does the theoretical uncertainty come from? To calculate the anomalous magnetic moment from theory, the contributions





The precession of a muon around the magnetic field is shown, left, and, right, the Feynman diagrams which represent the various contributions to the magnetic moment the muon are depicted. The hadronic vacuum polarisation is shown as a yellow bubble in the last contribution (APS/Alan Stonebraker).

from all other particles have to be taken into account. As it turns out, it is the contribution from the strong interactive particles called quarks and gluons that dominate the uncertainty in the theoretical prediction.

Giusti has been leading a PRACE project in which he has been designing and testing a new algorithm for computing this particular contribution, known as hadronic vacuum polarisation, to the anomalous magnetic moment of the muon. The aim is to try and bring the precision of the measurement of this contribution in line with the expected experimental error that will be achieved in next few years by Fermilab.

Our algorithm entirely factorises the propagation of the quark

“To meet this experimental error, we have to reach a precision of 0.2 per mille in our calculation,” says Giusti. “Using indirect computation based on other experimental results, it is possible now to achieve a precision of 0.6 per mille. With direct computation the error is much higher, but we aim to change this with our new algorithm.”

Direct computations of this particular contribution involve simulating a quark and anti-quark pair propagating through space and time, and calculating the so-called hadronic vacuum polarisation. This cannot be done on paper, as the theory of the strong interaction, known as quantum chromodynamics, cannot yet be solved analytically. Therefore, high-performance computing resources are used instead, using Monte Carlo simulations in which time and space are discretised into giant lattices consisting of millions of points mapped out on to thousands of processors in parallel. The novelty of Giusti’s algorithm is that it is able to subdivide the lattice into sub-blocks, so that computations of each region can be done independently. “Before, all of the computation would have had to be done together, meaning that to compute the propagation of the quark on one side, you would have to know what is on the other side. Our algorithm instead entirely factorises the propagation of the quark.”

This new algorithmic invention solves two problems. Before, to reduce the error of the measurement by a factor of 10 would have required an increase in computational power of 100. By factorising the computation completely, the increase in computational power needed is reduced to 10, which will be possible with upcoming pre-exascale and exascale computers. As well as this, the new algorithm will make parallelisation of the quark dynamic calculations much simpler.

The project finished in April 2021, and the results have been published in Physics Letters B and presented at ICHEP 2020 and at the Lattice 2021 conference at MIT. “The algorithmic development has now been completed thanks to the allocation from PRACE,” says Giusti. “Our next step now is to use this algorithm to carry out the actual computation of the hadronic vacuum polarisation contribution, which should take place in the next few years.”

Energy conversion and storage

Energetically excited states in heterogenous photocatalysts

Studying excitons and how they behave in certain materials is shedding light on the design of optimal materials that can be used in applications like energy conversion and energy storage. **Dr Sivan Refaely-Abramson** describes her work on this at the Weizmann Institute of Science in Israel as being at the intersection between physics, chemistry and materials science

When light shines on a material, something very exciting happens. Photons of light excite negatively charged electrons in the material to higher energy levels, leaving behind empty positive charges in the lower levels called holes. These negative electrons and positive holes can then be attracted to each other, forming what are known as excitons.

Dr Sivan Refaely-Abramson

In most materials, these excitons quickly collapse when the elevated electrons simply return to their original state and scatter the light energy. However, in some special materials, the excitons can remain stable and efficiently transfer the energy. Such materials are known as excitonic materials and are ideal for solar energy conversion and energy storage.

Investigating these kinds of materials is at the heart of Dr Sivan Refaely-Abramson's research, which lies at the intersection between physics, chemistry and materials science. After a PhD in which she developed methods for predicting properties of materials that could be used for organic photovoltaics, she then completed a postdoc at Berkeley where she learned advanced computational methods for understanding what happens when light interacts with such materials.

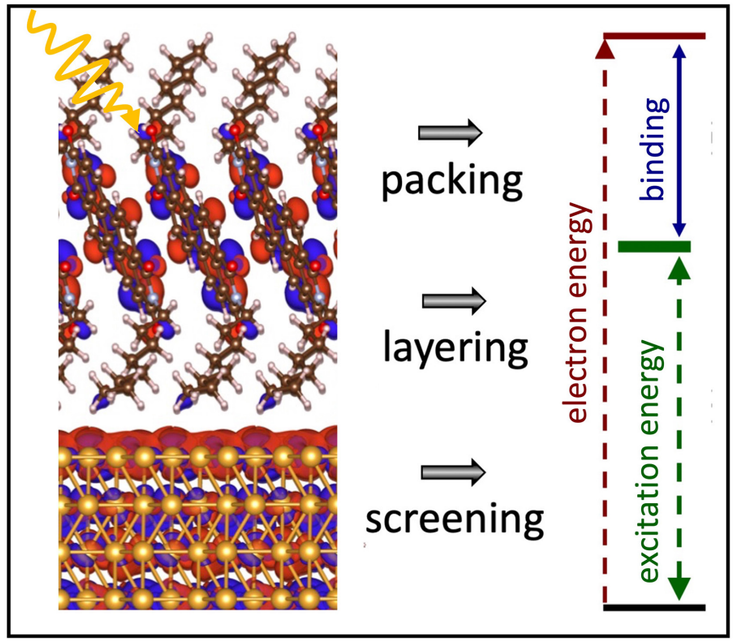
Refaely-Abramson now leads her own research group at the Weizmann Institute of Science in Israel, and the study of excitons and their properties makes up a significant part of their work. "We study how excited states in materials evolve over time, how they decay, and whether we can make them last longer," she says. "The properties of excitons are entirely dependent on the structure of the material they appear in, and if we are able to understand how and why these excitations can survive for a long time, it opens up the possibility of designing optimal materials for use in applications such as energy storage."

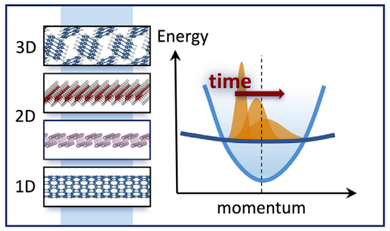
More information
http://www.weizmann.ac.il/materials/Sivan/home

HPC Resources awarded by PRACE
This project was awarded 30 000 000 core hours on MareNostrum 4 hosted by BSC, Spain.

In order to fine tune the structure of materials to improve the properties of excited states, predictive methods are needed. But to understand excited states at the predictive level, one must enter the realm of many-body quantum theory, an area of physics which provides a framework for understanding the collective behaviour of large numbers of interacting particles. While the underlying physical laws that govern the motion of individual particles are relatively simple, the study of larger numbers of particles is complicated by specific quantum phenomena that only manifest in such large systems.

While the most common way of dealing with these phenomena is to calculate an average estimation of their effects, Refaely-Abramson's group endeavours to provide a much more accurate depiction using what is known as many-body perturbation theory. This theory is an approximation of the many-body Schrödinger equation – an equation that provides the solution to understanding electronic properties in quantum problems, but which is impossible to solve in its complete form for systems of any significant size. So, how does this relate to excited states in materials? Many-body perturbation theory allows the group to gain a deeper understanding of excited states in materials by finding out how one particle scattering or moving effects the other particles in the system. These "response functions" are calculated using a code called BerkeleyGW, which when run on high-performance computers enables the researchers to predict the properties of energetically excited states in materials.





Above, the time propagation of energetically-excited quantum states depend on crystal momentum properties. A new theoretical approach demonstrates that crystal dimensionality dominates this propagation, allowing direct detection of materials' structure and symmetry through experimental measurement [Qiu et al., Nano Lett. 2021].

Left, an illustration of light excitation in an organic molecular crystal adsorbed on gold surface. The crystal molecular packing, the number of layers in it, and the environmental screening influence its electronic and excitation properties, as studied using advanced computational methods [Shunak et al., Front. Chem. 2021].

A recent PRACE project led by Refaely-Abramson aimed to study energetically excited states in heterogenous photocatalysts. The examined systems contain both organic and inorganic materials, and excited states occur at the interface of these materials which can then be used for energy conversion and storage. At present, most known photocatalysts are very inefficient, and although the reasons for this are understood, the right materials to improve this efficiency have not yet been discovered. Refaely-Abramson's group is now part of a global effort to try and find them. "Our aim is to create predictive structural design principles that will help in the discovery of more efficient photocatalysts."

The project has resulted in three publications. The first of these showed how the dynamics and lifetimes of excitons are related to crystal dimensionality in energy materials, and used these findings to present a way of predicting their structure and symmetry through experimental measurement. The second paper explored excited-state processes at organic-inorganic interfaces consisting of molecular crystals, in which molecules are packed together in a very specific orientation on a surface of gold. "We wanted to understand how the packing and symmetry associated with the dimensionality of the crystals affected the dynamical properties and nature of the excited states," says Refaely-Abramson. Finally, the third publication provided a detailed description of the electronic structures of excited states in a specific photovoltaic material.

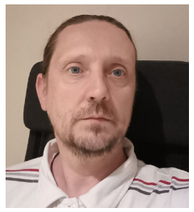
The allocation from PRACE has been crucial for the completion of the group's work. "Israel does not as yet have a Tier-0 supercomputer, but luckily we have had the opportunity to apply for access to PRACE resources," says Refaely-Abramson. "A big part of what makes the experience so good is the staff who are there to support you. In previous generations, I think it was thought that if you did computational work, you should take care of everything yourself, but this is actually not the best way to optimise such research. It is much better to work alongside technical experts, and I was very happy to find that PRACE had many such experts to help us along the way."

Computational earthquake seismology

Mapping the Earth's interior

Using a code that utilises the full knowledge of physics that dictates how waves propagate through the Earth, **Dr Vadim Monteiller** of CNRS has been using datasets gathered from the North Sea to create some of the most accurate images of the interior of the Earth to date, work that is now focusing on imaging a larger piece of the Earth in Japan to get information of the seismic hazards in that area

High-performance computing and computational seismology were made for each other. HPC feeds off big data and seismology is certainly rich in data. Put them together and a new world of possibilities for improving our understanding of geodynamics opens up.



Dr Vadim Monteiller

This is particularly true of computational earthquake seismology. Analysing ground motion scenarios for potential seismic events like earthquakes relies on being able to accurately image geological structures at multiple scales and on using the information buried in seismic big data records. Vadim Monteiller of CNRS is one of many seismologists who are now using the power of Tier-0 systems to be able to capture realistic images of the interior of the Earth using models that are only possible through enormous datasets. This work is a valuable advance for physics-based probabilistic seismic hazard assessment.

Monteiller has been studying these possibilities in a project using data from the North Sea on the Marconi100 GPU cluster at Cineca in Italy. "Our work involves looking at wave propagations," he explains. "When seismic activity occurs, the waves interact with complex geological structures inside the Earth, which can then be recorded at the Earth's surface. We use these records to image inside the Earth.

"It's a little like medical imaging, where you create an image of the whole body by studying the waves that propagate inside the body. We are doing the same with the Earth. Small meters and sensors are placed inside the Earth to create datasets of seismic activity, and we use these records to create images of the inside of the Earth."

A large dataset recorded using ocean-bottom seismometers in the North Sea above an oil field was used for Monteiller's PRACE project. The aim was to image the geological structures where oil and gas are extracted and create a precise image of the area, which required enormous computational power.

Monteiller and his team have developed a code called SPECFEM3D to carry out simulations of wave propagation inside the Earth to develop a model that explains the data gathered from the seismometers. "We started with an initial guess, compared the simulation with the data, and then slightly altered the model over and over again in order to explain the data better and better," he explains. "Tens of thousands of simulations were required to improve the model."

SPECFEM3D was developed along with several partners at CNRS, Princeton University in the USA and ETH in Switzerland. First ported to GPUs 10 years ago, it was developed and optimised for the PRACE project by Monteiller along with teams from the Barcelona Supercomputing Centre and Cineca in Italy, who analysed and modified it to speed it up. The resulting code was used to simulate wave propagation inside the Earth using a finite element method with high polynomial interpolation that made it very precise.

"We had a speedup of a factor of 300 going from CPUs to GPUs," says Monteiller. "It has made it possible to make precise images of the Earth, and since it is now a very fast and accurate code, we were also able to launch many simulations, especially with GPU clusters like Marconi100. This was the first time we were able to launch these simulations in such huge numbers."

More information

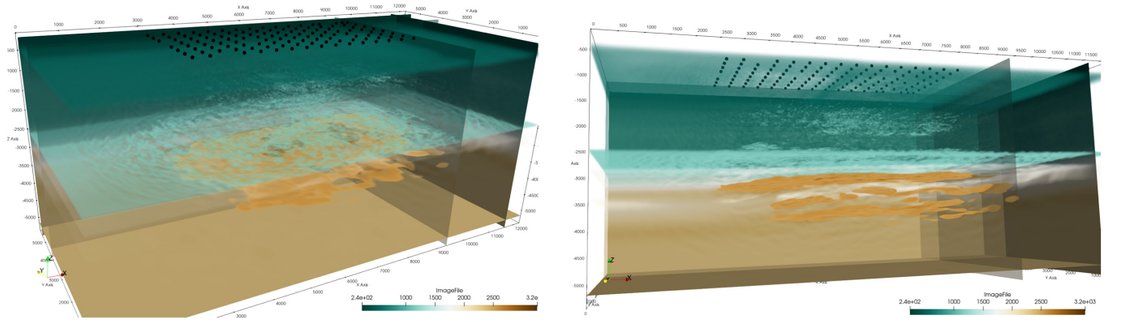
http://www.lma.cnrs-mrs.fr/

https://cheese-coe.eu/pilot/seismic-tomography

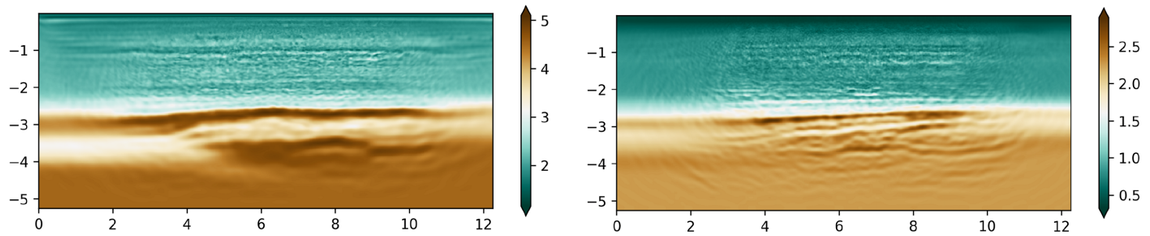
https://github.com/geodynamics/specfem3d

HPC Resources awarded by PRACE

This project was awarded 115 400 000 core hours on Marconi100, hosted by CINECA, Italy.



3D Geological structures recovered by 3D viscoelastic seismic Full Waveform Inversion. The data are recorded by 131 Ocean Bottom Seismometers in the North Sea (black dots).The color palette represents the different geological layers.



Detail of the different geological layers seen in vertical sections from the inverted 3D geological model (scale in kilometers)

The development of SPECFEM3D was done as part of the larger ChEESE project, which aims to create new codes for solid earth physics that can harness the power of upcoming pre-exascale and exascale supercomputers in Europe. This project has proven a valuable exercise in proving the capabilities of the code. "This is the first time we have done this type of computation," says Monteiller.

Previously, codes used for this kind of imaging used approximations of the actual physics at play. This project enabled the researchers to use their full knowledge of the physics of wave propagations, taking into account the viscoelastic properties of the Earth, as well as anisotropic properties, in which seismic waves propagate at different speeds depending on the direction in which they travel due to the crystalline properties of certain minerals. While this drastically increased the computational cost, it showed that it was possible to include this level of detail in simulations.

> *We need to understand the structure of the Earth to see how earthquakes are related to those structures*

Monteiller and his team are now working with the ChEESE project at a different scale. Instead of small-scale imaging like that used in this project on the North Sea, work is underway to image a larger piece of the Earth in Japan to get information of the seismic hazards in that area. "We need to understand the structure of the Earth there to see how earthquakes in the area are related to those structures," he says. "Now with this code, we have the technique to image at this larger scale.

"So, this code, developed as part of ChEESE and used for the first time with a very big dataset in this PRACE project, is now being used for more geodynamic purposes," concludes Monteiller.

Numerical relativity

Magnetic field amplification in binary neutron star mergers

Binary neutron star mergers are unique astrophysical laboratories for studying gravity due to the additional electromagnetic signals they produce. **Dr Carlos Palenzuela** of the University of the Balearic Islands is investigating the huge amplification of the magnetic field in these mergers to understand why it occurs and what relevance this amplified magnetic field has to the dynamics of the system

When Einstein first published his theory of general relativity in 1915 and propelled our understanding of gravity beyond Newtonian physics, any calculations of the theory's complex geometrical distortions of spacetime largely had to be done by hand. It would still be around half a century before the first supercomputers were built, marking the beginning of a paradigm shift in the way science is done.

Dr Carlos Palenzuela

Fast forward to today, and numerical relativity is one of the leading fields in supercomputing, pushing machines and software to their limits in the study of extreme astrophysical phenomena. Einstein's theory has remained the key method for describing such events, and the power of supercomputers has turbocharged it as a tool in the modern age of physics. The recent detection of gravitational waves – ripples of warped spacetime predicted by Einstein that are emitted by cataclysmic events – has opened up a wealth of new research avenues. In August 2017, simultaneous observations of gravitational and electromagnetic waves from the merging of two neutron stars – the densest known entities in the universe aside from black holes – marked the very first instance of such a multi-messenger astronomical event being observed.

When two neutron stars orbit each other closely, gravity causes them to spiral inward towards each other. When the two stars meet, their merger leads to the formation of either a more massive neutron star, or a black hole. As well as gravitational waves, this merger can also amplify the internal magnetic field of the stars, up to an intensity that is trillions of times stronger than that of Earth in a matter of one or two milliseconds. These events are believed to create short gamma-ray bursts and kilonovae, both of which emit electromagnetic radiation that can be detected from Earth.

While gravitational waves can provide information about the masses and velocities at play in such an event, the additional electromagnetic signals produced make binary neutron star mergers unique astrophysical laboratories for studying gravity, plasma physics and dense matter under extreme conditions. Dr Carlos Palenzuela of the University of the Balearic Islands has been leading a PRACE project investigating the huge amplification of the magnetic field that occurs in these mergers.

There are some ideas of why this amplification happens. Kelvin-Helmholtz instabilities – the same phenomena that cause waves to appear when wind blows over the surface of water – manifest when the two neutron stars ripple together, inducing turbulence that can trigger the magnetic field amplification. However, the scales at which these initial instabilities occur are so small as to be almost impossible to accurately model using even the largest computing resources.

"What we proposed in this project was to use high resolution and high order numerical schemes alongside a technique called large eddy simulations which is especially designed to examine turbulent regimes," says Palenzuela. "We hoped that the combination of these tools would allow us to capture the turbulent stage with enough accuracy to answer questions about why the magnetic field is amplified, what form the magnetic field takes in terms of shape and size, and what the relevance of this amplified magnetic field has to the dynamics of the system."

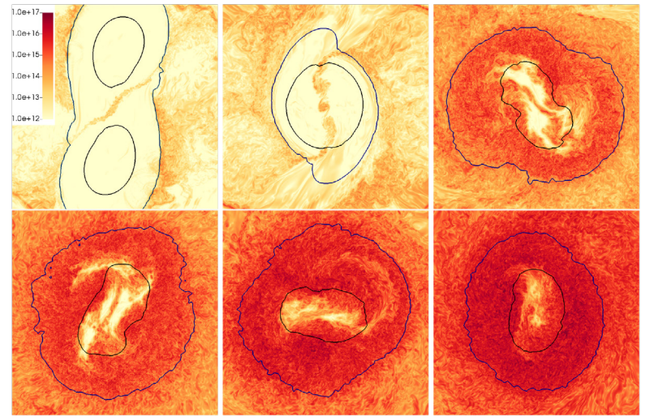
More information

http://iac3.uib.es/

https://bitbucket.org/iac3/simflowny/wiki/Home

HPC Resources awarded by PRACE

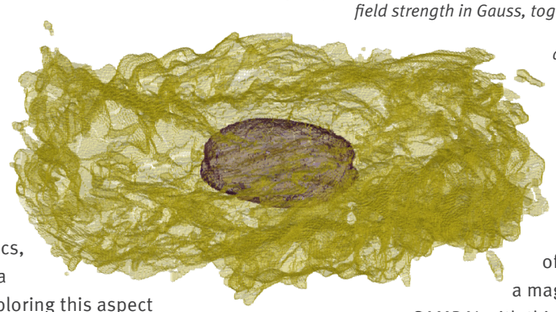
This project was awarded 14 200 000 core hours on MareNostrum 4, hosted by BSC, Spain.



Merger of neutron stars. Snapshots at representative times displaying the magnetic field strength in Gauss, together with density isosurfaces representing the core and the envelope of the star. The amplification is driven mainly by the Kelvin-Helmholtz instability, that induces a turbulent stage which is accurately captured by using Large-Eddy Simulations with high resolution.

The simulations, which show few tens of milliseconds of a binary neutron star merger, examine a number of different variables within the system. "At the most basic level, we are computing the energies involved in the system: the rotational kinetic energy of the stars and the magnetic energy being produced, as well as the poloidal and toroidal components of the magnetic field. We also look at the entire star envelope – the larger area of gas that contains the whole system – to see how it grows over time."

On top of this, Palenzuela's team also examine the spectral density of the system, breaking down the distribution of energy into the various discrete frequencies produced. "In principle, from what we know about the physics, we expect the spectra to look a certain way," he explains. "Exploring this aspect is the costliest part of our analysis, as it involves performing Fourier transformations in 3D with thousands of points in each direction. This part of our calculations has to be parallelized efficiently, as there are no machines today that have enough memory to do it directly."



Merger of neutron stars. Density isosurfaces just after the merger of two neutron stars. The collision produces a rotating massive remnant that will eventually settle down into a spinning neutron star. The isosurfaces represent roughly the core and envelope of the remnant.

Through the past decades, a number of codes have been developed – with varying degrees of success – for carrying out such simulations, mostly designed by physicists rather than computer engineers. "We decided to take a different approach, using a public infrastructure called SAMRAI developed by experts at the Livermore Laboratories in the USA that takes care of issues such as parallelization and scaling that, as physicists, we know little about.

"Then, on top of that infrastructure, we run our own software called SIMFLOWNY that uses high order numerical schemes to solve the Einstein equations for describing compact objects such as neutron stars, as well as high-resolution shock-capturing methods for solving the magnetohydrodynamic equations, because the matter of the neutron star is described as a magnetized perfect fluid. By joining SAMRAI with this software of our own, we have created a new code called MHDUET."

Preliminary results of the project have surprised some colleagues in the community, and the effects of the initial magnetic field on the final stage after the merger remains a disputed topic. As such, Palenzuela is now looking to carry out several similar simulations with different initial configurations to try and resolve the debate. "My impression is that because of the existence of this intermediate turbulent stage, all memory of the initial state of the system will be lost, making the final result independent of the initial magnetic field," he says. "Of course, future work will also depend on what happens in our final high-resolution simulations. One option would be to continue the simulations beyond the first tens of milliseconds to reach the stage where the system collapses into a black hole. When this happens, an accretion disk of material forms around the black hole which is largely responsible for the appearance of jet outflows and short gamma ray bursts that power electromagnetic emissions detectable from Earth."

Simulating turbulent flows

Refining the models of small-scale turbulence

Kolmogorov's eighty-year-old phenomenological observations of turbulent flows remain the cornerstone of research into turbulence, but computational work led by **Professor Alessandra Sabina Lanotte** has challenged some of these predictions and will help improve the predictive power of simulations of the ocean and atmosphere

The eddies and whorls seen in the flow of fluids have long been a source of fascination for scientists, the simultaneously coherent and unpredictable movements long alluding any unified theory to describe them. Collectively, this unpredictable motion is referred to as turbulence.

Prefessor Alessandra Sabina Lanotte

As there is still no theory derived from principle that can be used to describe turbulent flows, researchers in this domain instead rely on phenomenological models. The first of these was introduced in the 1940s by Soviet scientist Andrey Kolmogorov which, as of today, remains the reference theory for describing turbulent flows, in applications ranging from engineering to atmospheric modelling and medicine.

Over time, people have tried to challenge Kolmogorov's theory to see if it holds true in the face of rigorous testing. One of the building blocks of the theory is that the energy distribution of turbulent flows all follow a similar pattern, known as the –5/3 power law. But while Kolmogorov originally derived this rule in a simple setup, real turbulent flows tend to be more complex, and it is in these more complex situations that the rule begins to falter.

To be able to challenge Kolmogorov's predictions, one of two routes must be taken. Carrying out field experiments, for example taking real measurements of turbulence in the atmosphere or ocean, is one of these. The other involves using high-performance computers to do extremely large direct numerical simulations, and this is the path down which Professor Alessandra Sabina Lanotte's career has taken her.

As a theoretical physicist specialising in numerical simulations of fluid dynamics problems, Lanotte has a particular interest in investigating turbulent flows. "The disorder and chaos of turbulence means that it is as yet impossible to know for certain the characteristics of a flow at any specific moment in time or point in space," she says. "Instead, what we do is to try and work out the average properties of the flow, as well as what happens at the extremities of the energy distribution – the rare events. These rare events are important because they are often associated with failure in engineering, for example when wind turbines break in extreme conditions."

In a recent PRACE project, Lanotte simulated turbulent flows to gain a better understanding of such flows seen in the ocean. The simulations looked at water in elongated geometries much larger on the horizontal axis than the vertical axis, much like the ocean. Effects such as rotation and stratification were then introduced, either matching the levels seen in the ocean or pushing them to their upper limits to gain a fuller understanding of the resulting turbulent phenomena.

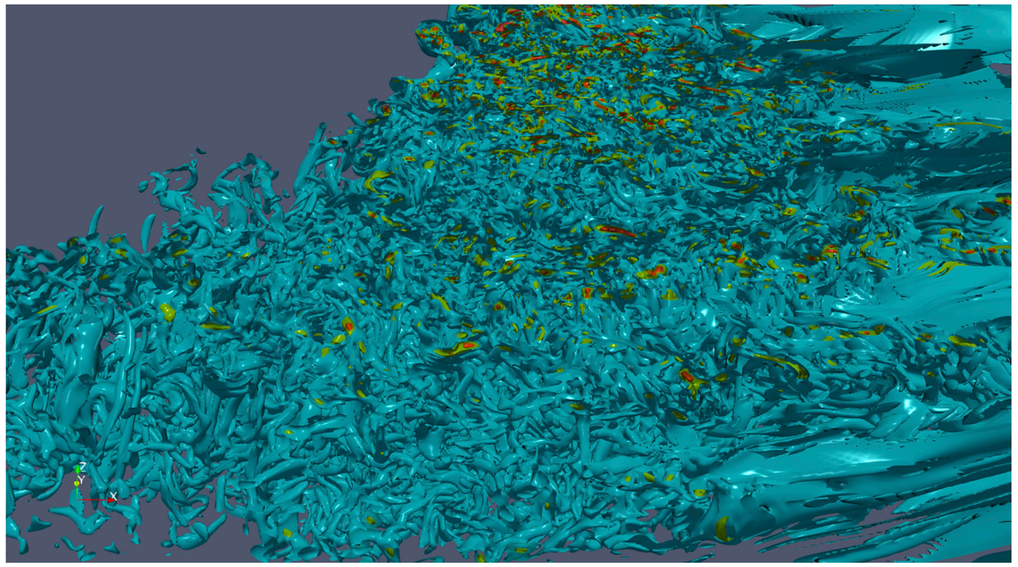
"The difference between our work and what had been done previously by other researchers was that we did not use standard forcing," says Lanotte. "All turbulent flows need energy injected into them to keep them alive, otherwise the energy in the flow eventually degrades into heat and the turbulence disappears. The problem is that it is usually impossible to distinguish the effects of the waves and the vortices in such forcing. What we did was to inject these types of energy separately to disentangle their roles in the turbulent flow."

More information

https://alanotte.weebly.com/

HPC Resources awarded by PRACE

This project was awarded 56 000 000 on Marconi, hosted by KNL CINECA, Italy.

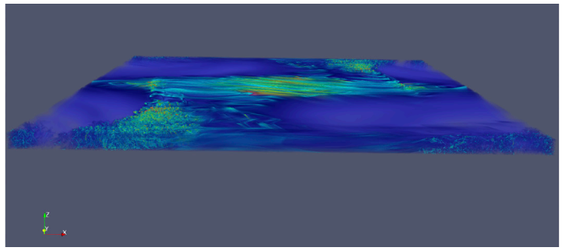


A zoom into the most intense turbulent structures

Lanotte's team is still analysing their results, so they still do not know whether the Kolmogorov spectrum is always maintained, or if there are deviations away from it. "Working on this project has been a struggle at times due to the pandemic – I never once saw the students I was working with throughout the whole course of the project!", says Lanotte. "But the results we have obtained so far have been collated into a PhD thesis by Vincenzo De Toma, and hopefully we will then be able to have some papers published."

Looking forward, one of the team's main goals is to refine the models of small-scale turbulence used in meteorology and oceanography to provide better overall predictive powers. "When running global circulation simulations to describe the ocean and the atmosphere, whether it be for short-term weather forecasting or for predicting long-term climate change, you can never fully simulate all of the motions at all scales. You have lower limits, and beyond them you must use models.

"All of the models used in such cases are based on Kolmogorov's laws, so if we are able to correct these somehow, or provide some pointers as to when and where these laws might start to break down, then we can help improve the overall predictive powers of these types of simulation. We are working alongside an oceanographer from the United States who is helping us to integrate our work into such simulations."



Amplitude of a turbulent velocity field confined in a thin layer

Lanotte believes that the power and importance of numerical simulations has yet to be fully appreciated in the minds of scientists and the wider public. "I work in an institute where most of the people are experimentalists," she says. "When I talk to them about numerical simulations, I often get the impression that they think these take a couple of minutes on my desktop computer! It is important for the next generation of scientists to understand that carrying out numerical simulations on Tier-0 resources like those provided by PRACE is a huge undertaking, as challenging as the largest lab experiments. In the future, I think students need to be introduced to this kind of work at the undergraduate level."

Dry eye syndrome

How blinking affects the tear film lipid layer in the eye

Dry eye syndrome is a painful condition affecting millions of people throughout the world and is caused by the evaporation of tear fluid from the eye surface. What causes this evaporation is the focus of a PRACE project led by **Professor Ilpo Vattulainen** and a team at the University of Helsinki, with the work concentrating on the lipid molecules on the eye surface and how their behaviour is affected by blinking

Dry eye syndrome (DES) is one of the most common diseases of the eye, estimated to affect more than 400 million people around the world. The condition is caused by excessive evaporation of tear fluid from the surface of the eyes, leaving them dry and scratchy and often causing blurred vision. It can be exacerbated by prolonged interaction with computer screens and in air-conditioned rooms where the atmosphere is very dry.

Prefessorn Ilpo Vattulainen

It is not clear why some people suffer with DES and others do not. Treatments are available in the form of eye drops, but these need to be applied regularly to ease the recurring symptoms. If left untreated, the condition can in rare cases lead to blindness.

What is known about DES is that the excessive evaporation of tear fluid is linked to the impaired function of the tear film lipid layer (TFLL) that covers the watery film over the eyes. The TFLL keeps the eyes moist by providing this surface layer of fluid with resistance to evaporation. How it does this and why it sometimes fails has been the focus of a PRACE project led by Professor Ilpo Vattulainen and his team at the University of Helsinki.

Vattulainen specialises in the field of biological physics, using theoretical and computational techniques to explore the underlying physical principles that govern the behaviour of biological systems. With a particular focus on lipid membranes and the ways that they modulate key biological processes, his group has been applying its knowledge and methods to try and understand the mechanisms behind the evaporation resistance of the TFLL.

Previous simulation work by the group had shown how wax esters, lipid molecules that are present at the surface of the eye in large amounts, are able to extensively slow down water evaporation. However, these simulations looked at the TFLL in a state of equilibrium, which is not a realistic representation of what occurs in the eye, as Vattulainen explains: “When looking at a computer display, you blink your eyes every ten seconds. Each time this happens, the lipid layers on the surface of your eyes are compressed and then gradually expand afterwards.

“The question we wanted to answer is how this process of compression and expansion, which creates a constant state of non-equilibrium, affects the reorganisation of the lipid layers, and how this in turn is linked to water evaporation.”

The team simulated this non-equilibrium process thoroughly, performing many repeats under various conditions. “We looked at how evaporation changed in systems with wax esters compared to those without, and also did the same for other similar lipids such as cholesteryl esters. Lipid by lipid, we checked the importance of these for the stability of the lipid layers at the surface of the eye, checking their importance in retarding water evaporation while trying to simulate the layers in as realistic conditions as possible.”

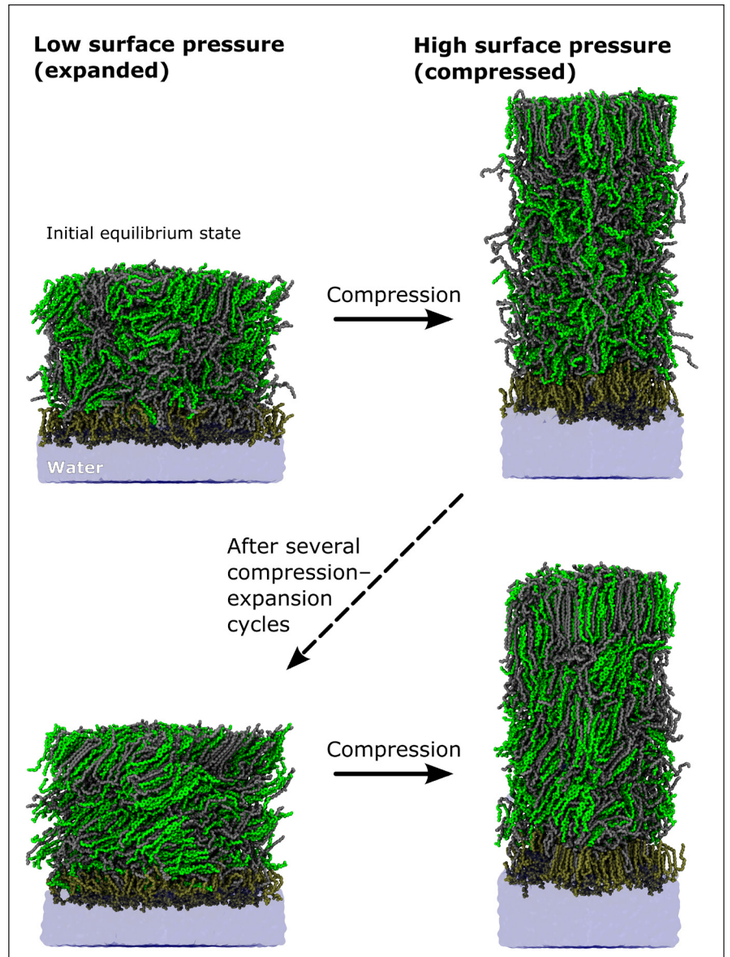
These atom-scale molecular dynamics simulations have provided the first-ever atomistic view into the non-equilibrium properties of the TFLL. The team discovered that through blinking, cholesteryl esters and wax esters in the non-polar lipid bulk form multilayered crystal-like structures that act as an evaporation resistant barrier. Polar lipids also settle against the water, spreading the TFLL over the layer of moisture. (See figure 1)

It was also discovered that while in a disordered lipid structure, water molecules have more ways to escape from the water phase and travel into the air, the highly-packed, crystal-like structure of the non-polar lipid components acts as an effective barrier, retarding water evaporation. The structure of the bulk phase of the TFLL is controlled by lipid composition and thermodynamic conditions.

“The big piece of news to emerge from this project is that the non-equilibrium behaviour is quite different to the equilibrium behaviour that occurs without any blinking,” says Vattulainen. “In a practical sense, this could lead to eye drops for DES that contain wax esters, which they don’t at the moment. This would mean that the drops would last longer and wouldn’t need to be applied every hour.”

A number of further lines of research could be explored to follow up this project. While the TFLLs studied simulated ranged from 20-30 nanometres in thickness, they tend to be closer to 100 nanometres in reality. This would however require much larger computing resources. As well as this, the simulations did not take into account any of the proteins that are present in real TFLLs. “A number of surfactant proteins that are known to exist in the lung, including those that enable oxygen permeation into the blood, are also found in the TFLL,” says Vattulainen. “So far, no experimental work or simulations have managed to explain the presence of these proteins in the eye.”

Vattulainen and his Helsinki team are confident that progress in understanding DES will continue thanks to LUMI, a new petascale machine under construction in Kajaani, Finland, of which Finland will own 25% of the computing capacity. “But when we applied to PRACE for this project, our own computing resources were quite small,” he says, “so we were extremely happy that PRACE decided to support us.”



The compression–expansion cycles of the tear fluid lipid layer (TFLL) explored through atom-scale molecular dynamics simulations provide the first ever atomistic view into the non-equilibrium properties of the TFLL. The systems start from an equilibrated expanded state at low surface pressure. They are quickly compressed to high surface pressure with low area per lipid, and again expanded to a low surface pressure to imitate blinking. After several cycles of subsequent compression and expansion, cholesteryl esters (light green) and wax esters (gray) in the non-polar lipid bulk form multilayered crystal-like structures that act as an evaporation resistant barrier, retarding water evaporation. Polar lipids (dark green) settle against the water, spreading the TFLL over the aqueous phase. (Image: Juho Liekkinen /Vattulainen group.)

More information
https://www2.helsinki.fi/en/researchgroups/biophysics

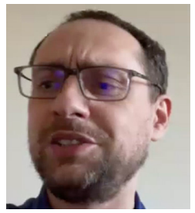
HPC Resources awarded by PRACE
This project was awarded 67 000 000 core hours on Joliot-Curie in Rome, hosted by GENCI/CEA, France.

Colliding quantum vortices

Understanding the superfluid interior of neutron stars

It is only by using high-performance computers that **Dr Gabriel Wlazłowski** of the Warsaw University of Technology has been able to advance our understanding of neutron stars and how quantum vortices colliding inside them are responsible for speeding up of their rotational frequency. He believes this work is just starting and with the advent of exascale systems much larger simulations will be possible

It is hard to overstate the influence of quantum mechanics on our understanding of the world – it rewrote rules that had stood for over 200 years and is the foundation upon which much of our knowledge in science and technology today is built. But its oversized presence belies its subtle nature. Its more curious effects manifest almost exclusively at the atomic level and, at the level that we experience the world, barely describes the world any differently than classical physics.



Dr Gabriel Wlazłowski

However, there are a few instances where the strangeness of quantum mechanical effects can be observed with the naked eye. A superfluid is an exotic state of matter that lacks viscosity, the internal friction that allows normal fluids to resist and cause motion. This lack of viscosity bestows all sorts of weird properties upon superfluids, allowing them to climb up the walls of their containers or even pass through thin solid materials.

Dr Gabriel Wlazłowski of the Warsaw University of Technology has been developing a version of density functional theory that can be used to accurately describe strongly interacting systems such as superfluids. A recent PRACE project aimed to test this method in the context of two physical systems: ultracold atomic gases and neutron star crusts. Although seemingly very different, both are described by remarkably similar microscopic theories and share similar superfluid properties.

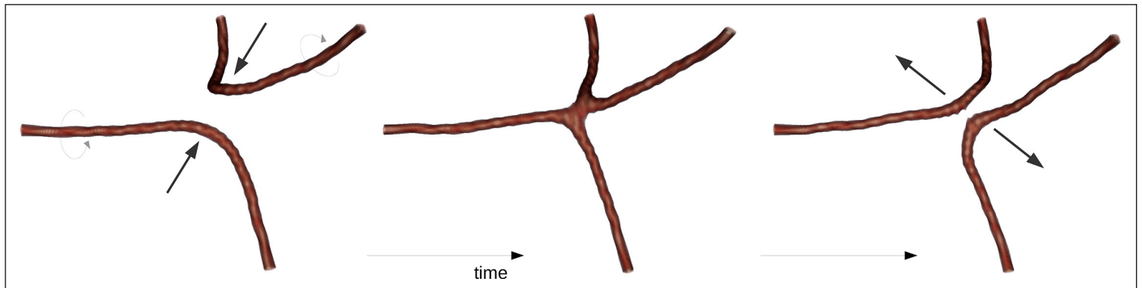
Neutron stars – the collapsed cores of massive giant superstars that, aside from black holes, are the densest known stellar objects in the universe – are one of the targets for Wlazłowski's methods. Due to the impossibility of studying such entities experimentally, much of what is known about neutron stars today has been found through simulations. Some phenomena recently observed in neutron stars have led some to believe that they may be superfluid, but in order to develop the computational methods to study this, they must first be tested on smaller, known systems.

Ultracold atomic gases that, like many suspect neutron stars to be on the inside, are superfluid. However, unlike neutron stars, it is possible to study ultracold atomic gases in a laboratory setting. Recent work from experimentalists looked at rotating and strongly-interacting gas in its superfluid state, cooled down to nanokelvin temperatures just above absolute zero. Normally when a fluid is put into rotation, like when it is stirred, it ceases to rotate due to angular momentum transferred via viscosity, which can be simply understood as a kind of internal friction. Superfluids have zero viscosity, so angular momentum is instead carried by what are known as quantum vortices. They can rotate forever. Wlazłowski has been trying to replicate the quantum vortices measured in experiments to validate his computational methods.

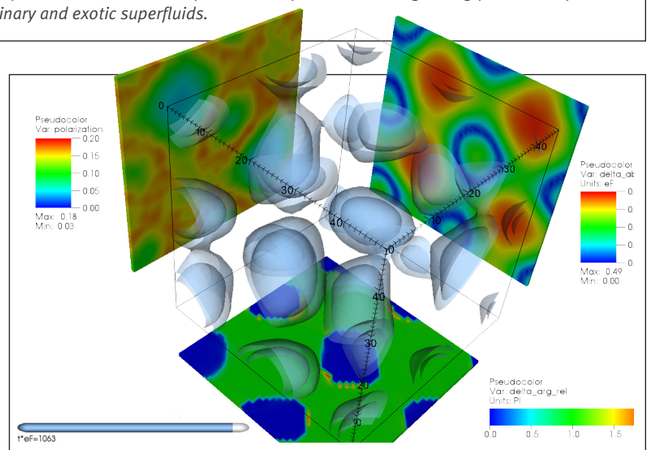
Wlazłowski's simulations have been able to show in great detail the process of quantum vortices colliding, a process known as reconnection. It is believed that quantum vortices are responsible for a phenomenon observed in neutron stars in which their rotational frequency periodically speeds up. "There is a hypothesised model that explains this phenomenon in which the interior of the neutron star is presumed to be a superfluid," says Wlazłowski. "When many quantum vortices reorganise simultaneously in this giant mass of superfluid, it manifests at the macroscopic level as this increase in rotational speed. In the future, we hope to be able to study these systems in more detail using the methods we have been refining in this project."

More information
http://wlazlowski.fizyka.pw.edu.pl

HPC Resources awarded by PRACE
This project was awarded 85 300 000 core hours on Piz Daint, hosted by CSCS, Switzerland.



Collision of two quantum vortices. In the collision, the vortices approach each other, merge locally and reconnect, leading to a new topological configuration. Although the phenomenon is a very nonlinear process, it turns out that its dynamics is universal close to the reconnection point. Having access to Tier-0 granted by PRACE, we confirmed that it proceeds in the same way in various systems, including strongly and weakly interacting Fermi superfluids, Bose-Einstein condensates, ordinary and exotic superfluids.



Exotic state in Fermionic superfluid: the spin-imbalanced gas of strongly interacting particles spontaneously creates localized impurities. The characteristic feature is the presence of the nodal surface (blue contours) of the pairing field at which the order parameter changes its phase by π (delta_arg_rel panel). The spin polarization reaches the maximum in the vicinity of the nodal surface (see polarization panel). The impurities, we dubbed ferrons, can form various structures, in the given example they organize similarly to ions in solid-state. The existence of ferrons has been predicted numerically and awaits for experimental conformation.

As well as trying to replicate experimental data using their methods, Wlazłowski and his team have also used their PRACE allocation to work the other way, making predictions that can then be checked by experimental teams. One of the predictions they have made is the existence of a novel superfluid state in which small pockets of the fluid have much higher density. Such states are referred to as supersolids. Historically, the development of density functional theory has strongly correlated with development of high-performance computing. It took teraflop performance for the theory to become useful for quantum chemistry and solid-state physics applications.

To study strongly interacting systems such as superfluids, the computational need is a thousand times greater, but this has now become possible with current Tier-0 systems such as Piz Daint, on which Wlazłowski's work was carried out. "Our work in this project is really just the beginning," he says. "We can now see that it is possible to apply this method on such systems, so we can now start working on refining the methods so we can trust the results, and also begin planning for the possibilities of exascale systems. Right now, we simulate systems at a much smaller scale than experimental set-ups but, with the dawn of exascale systems, we should be able to simulate them directly."

Wlazłowski's team has published a number of papers based on this work using PRACE resources that he believes will showcase the ability of high-performance computing to address such topics to the wider scientific community. "In the long term, we want to start building a community of people gathered around these methods," he says. "We have released our codes in the form of open-source software, and eventually we would like to create a toolkit available to all that will be designed specifically for studying the interiors of neutron stars."

Generation IV nuclear reactors

Fluid dynamics of liquid metal coolants in nuclear reactors

The next generation of nuclear reactors will generate huge amounts of heat at the core and so require new cooling methods. **Dr Lilla Koloszar** of the von Karman Institute for Fluid Dynamics has been testing methods that will aid the development of this new generation of reactors

The world of nuclear power has come a long way since Chicago Pile-1, the first ever nuclear reactor, was built in 1942 by Nobel Prize winner Enrico Fermi. Most of the reactors in use around the world today are what are known as Generation II reactors, while Generation III reactors are just now starting to come into operation. Naturally, forward-thinking researchers have already begun working on designs for Generation IV reactors, with the aim of improving safety, sustainability, efficiency, and cost.

Dr Lilla Koloszar

The Belgian Nuclear Research Centre (SCK CEN) is currently designing a Generation IV reactor called MYRRHA which is cooled by a liquid metal called lead-bismuth eutectic (LBE). Dr Lilla Koloszar of the von Karman Institute for Fluid Dynamics specialises in studying the flow of such liquid metals, and has been leading a PRACE project in collaboration with SCK CEN in order to analyse the cooling system of this new nuclear reactor with high resolution in space and time. This will provide useful information to the nuclear researchers and engineers still working on the design of the reactor.

One of the main aims for the MYRRHA reactor is to be able to post-process the nuclear waste produced so that its half-life – a measure of how long the waste remains radioactive – is reduced from the order of hundreds of thousands of years to just hundreds of years. “In order to achieve this kind of reduction, you need a very compact core,” says Koloszar. “But with such a compact core you generate huge amounts of heat in a localised area which needs to be cooled efficiently, and this is impossible with conventional fluids. That is why we have to use liquid metals such as LBE.”

More information
https://www.vki.ac.be

HPC Resources awarded by PRACE

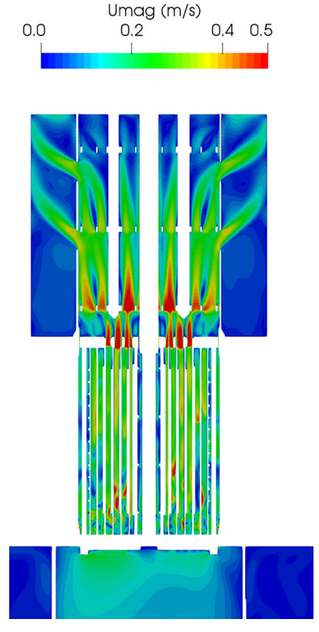
This project was awarded 30 000 000 core hours on Joliot-Curie Rome, hosted by GENCI at CEA, France.

Using liquid metals for cooling is a relatively new concept that at present is only used in Russian nuclear submarines at a much smaller scale than proposed here. “We are carrying out validation and verification of our computational fluid dynamics code by comparing it with the experimental data,” says Koloszar. “At this stage, a scaled-down version of the reactor called E-SCAPE that is one sixth of the full size of MYRRHA has been built. It is heated by electricity rather than by nuclear power, and in this project we are carrying out simulations that can be compared with readings from the model to help with validation of the code.”

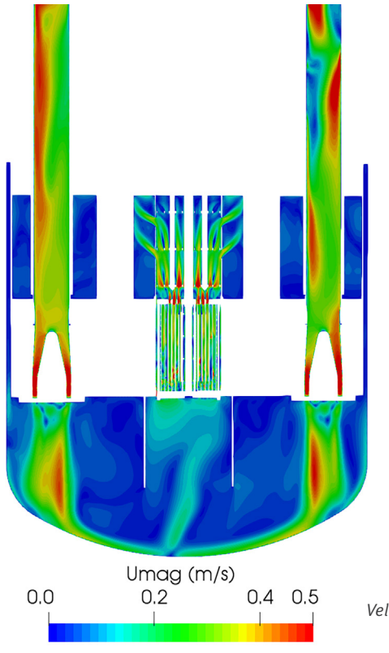
Despite only being one sixth of the size of the proposed reactor, the experimental setup is still huge, with a diameter of over one metre. The pool of liquid metal used to cool it is extremely challenging to simulate accurately, and it is only thanks to HPC resources provided by PRACE that Koloszar’s team are able to simulate this pool both in operating conditions and in more transient conditions when the temperature of the coolant changes due to changes in the reactor output.

To do these simulations, a solver family called called myrrhaFoam was used, which is a variant of the open-source OpenFOAM simulation platform. These codes were developed through several years of collaboration between the von Karman Institute for Fluid Dynamics and SCK CEN. “We customised this code to be able to deal with liquid metals, because the general code had some shortcomings both from the nuclear side and from the liquid metal side,” says Koloszar.

After beginning the project, Koloszar and her team



Velocity field in the core of E-SCAPE.



Velocity filed in the mid-plane of E-SCAPE.

realised that the meshes needed to simulate the system were much larger than originally estimated. Despite this, they were able to achieve everything that they set out to do. “The support we received working on the Joliot Currie cluster hosted by GENCI at CEA was amazing,” she says. “We had many difficulties with compiling, and it is only thanks to this support that we were able to finish our work in time.”

With the E-SCAPE system, the flow of the fluid in the system could not be directly measured. Instead, measurements of the thermal field were taken, and these were then compared with the simulations to see if they matched up. “We were unsure if our code would be able to grasp the 3D nature of the flow, especially in what we call natural convection cases,” says Koloszar. “I must admit that the comparisons with the thermal field measurements were impressive. This showed that our simulations were almost certainly providing an accurate depiction of the flow field within E-SCAPE.”

The researchers are now involved in two ongoing European research projects that aim to investigate potential transient conditions and accidents in the MYRRHA reactor. “We hope to be able to continue using Tier-0 resources from PRACE for this further work, as simulations of transient conditions will be even more demanding than those performed in this project.”

Such a compact core generates huge amounts of heat in a localised area, which needs to be cooled efficiently

An interesting aspect of this project was that it was all carried out using low-order codes. “Usually in my field, direct numerical simulations would be done with highly specific codes,” says Koloszar. “What we have shown is that there is now a real need for high-performance computing beyond the world of academia and highly-specialised codes, and also that these low-order codes can actually scale very well on these huge problems.

“Working with Tier-0 resources has been an amazing experience. Usually with such huge geometries, you start the simulation and then come back to get the result one month later. Instead, we were able to run on hundreds of nodes consisting of thousands of processors and get our results back in a few days. Being in a situation where your brain and your practical capabilities are the bottleneck rather than the simulation time is an excellent challenge. As researchers, we always want to develop to become better and better, so when we are challenged like this we are happy!”

Simulating solar magnetism

New understanding of both large and small-scale solar dynamos

Increasingly high-resolution and theoretically advanced simulations are providing a greater understanding of the sun by enabling the simultaneous capture of the two main constituents of the solar dynamo - the small and large-scale solar dynamos. Now, in a PRACE project led by Professor **Maarit Käpylä** of Aalto University, two breakthroughs have been made that may lead to us being able to understand the solar dynamo once and for all

The blinding white disk in the sky we call the sun – the source of light and life on Earth – is a colossal, writhing ball of intensely hot plasma. Its surface spits with arcs of fire that extend for thousands of kilometers into space, caused by the fact that the sun is a giant magnetic star made of material that moves in concert with the laws of electromagnetism

Professor Maarit Käpylä

The magnetism of the sun has a huge influence on our solar system, even causing visible effects on Earth in the form of auroras. It is produced by an enigmatic process called the solar dynamo which, to date, numerical models have only had moderate success in accurately describing. Overly simplistic models that do not take into account many of the processes known to occur in the sun have meant that a rough qualitative description has been the best that simulations have been able to offer.

Recently, more accurate observations of the sun have provided invaluable information to those working on simulations of the sun. The increasingly high-resolution images of the solar surface have revealed a seemingly unending depth of smaller and smaller magnetic structures, indicating that the solar plasma is not only intensively turbulent, but that this turbulence is likely an important constituent of solar magnetism.

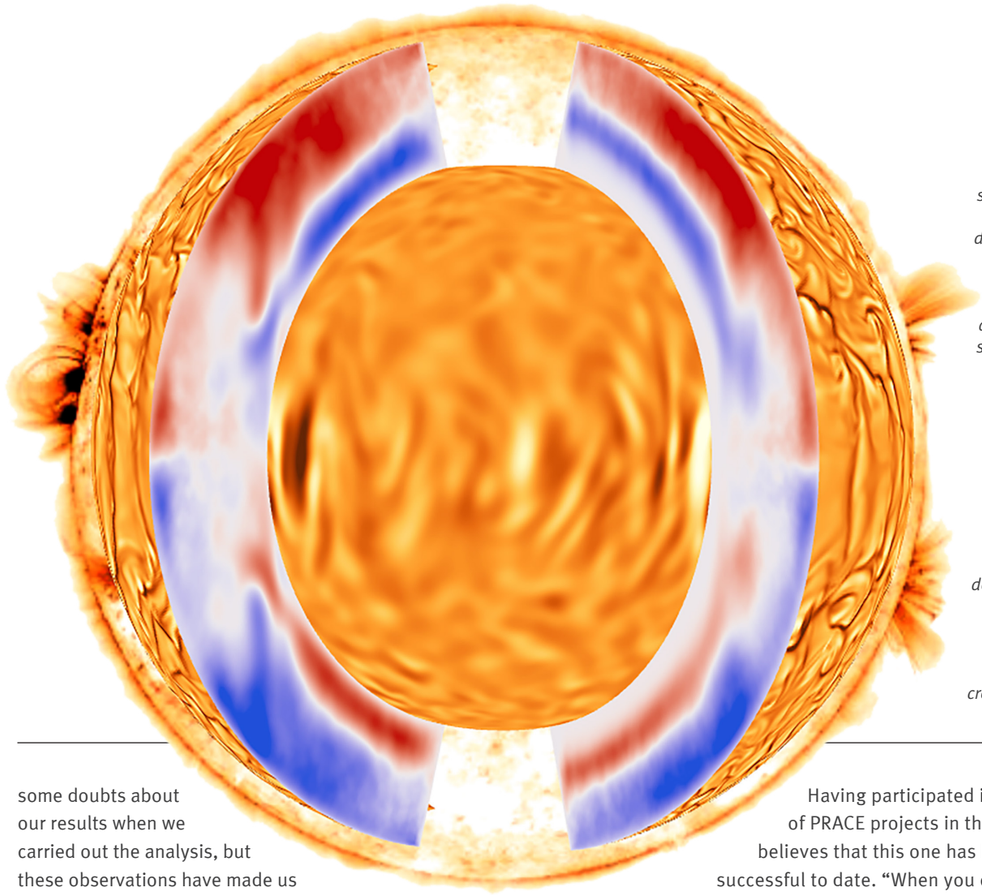
Recently, top global dynamo modelling groups around the world have reached the point at which they can simultaneously capture the two main constituents of the solar dynamo, known as the large-scale and small-scale dynamos. Professor Maarit Käpylä of Aalto University has been leading a PRACE project with the objective of improving upon current numerical models to provide answers to the many questions and controversies that surround the solar dynamo. “The simplest upgrade that we were able to implement, thanks to the Tier-0 resources provided by PRACE, was to run the simulations at a higher resolution so that we could gain a better understanding of the turbulent flows and magnetic fields at play,” she says.

Aside from higher resolution, one of the major improvements made in the project was to remove over-simplistic models of heat conduction and instead allow it to evolve as a function of the density and temperature of the system. In the solar convection zone – the outermost layer of the solar interior – magnetism is generated in a cyclic fashion due to the motion of plasma. This is known as the large-scale dynamo. In the majority of previous models, the solar convection zone was assumed to be convective at all depths, but the new concept modelled by the team led by Käpylä removes this assumption.

As it turns out, tweaking the model to allow convection to evolve more freely had a big effect on the dynamics of the system. “With our improved model, we saw a layer at the bottom of the ‘convection’ zone that was not at all convective but still transported heat towards the surface – with entirely different properties than seen in previous simulations,” says Käpylä. “Interestingly, subsequent observational data published very recently seems to indicate that these layers do in fact exist. We had some doubts about our results when we carried out the analysis, but these observations have made us realise that we may have discovered something important in terms of magnetic field evolution in the sun.”

More information
https://www.aalto.fi/en/department-of-computer-science/astroinformatics

HPC Resources awarded by PRACE
This project was awarded 57 000 000 core hours on SuperMUC-NG, hosted by LRZ, Germany.



A volume rendering of global convective dynamo simulations. Colours on the two spherical surfaces represent the radial velocity close to the surface and the bottom of the simulation domain. The meridional cuts show a quantity obtained as a result of an elaborate data analysis chain from the simulations, describing how the convective turbulence takes part in the dynamo process. In the high-resolution simulations with improved heat conduction treatment, thick inversion layers are seen (red colour changing to blue with depth). The background image is from an instrument on board the Solar Dynamics Observatory. Image credit Dr. Ameya Prabhu.

As well as the large-scale dynamo caused by the motion of plasma in the solar convection zone, there exists another dynamo instability called the small-scale dynamo which generates a non-cyclic, fluctuating component to the magnetic field of the sun. Until this project, the extent to which this small-scale dynamo occurred was not well known, but the increase in resolution and turbulence in these simulations enabled the researchers to confirm that this instability may well play an important role in the solar dynamo.

“Now that we have been able to locate and isolate the amplification of small-scale magnetic fields, we will be looking to study the influence of this effect on the overall solar dynamics,” says Käpylä. “It has been said that to truly understand the solar dynamo, this secondary instability must be accounted for, so we are quite excited that we will finally be able to investigate it properly.”

Having participated in a number of PRACE projects in the past, Käpylä believes that this one has been her most successful to date. “When you carry out these extremely large simulations, you cannot store all of the data from them,” she says.

“Instead, you have to harvest what you think is important and then move on. Consequently, in the aftermath you often have regrets and think about how you might have done things differently, but in this project, everything went just as planned.”

As the relentless march towards larger and more powerful computers and data centres continues, Käpylä believes that there is a need for more investment into optimising the codes that are used on them.

“The world of high-performance computing is moving fast, and in the last few years we have already had to deal with our first major paradigm shift from using CPUs to GPUs,” she says. “With the advent of quantum computing next in line, we need to ensure that we are ready with algorithms that can adequately use these technologies.”

Hybrid improper ferroelectric materials

Enhancing ferroelectric and magnetic properties of materials

Perovskites are versatile materials that have a wide variety of characteristics and can be used as building blocks to create more complex structures that have several interesting properties. In their PRACE project, **Dr João Pedro Esteves de Araújo** and his team at the University of Porto have been investigating these materials and looking in particular at negative thermal expansion, which has a number of potential applications including high-precision optical and microelectronic devices

Dr João Pedro Esteves de Araújo of the University of Porto leads a team of condensed matter physics researchers in the study of complex materials with useful properties, combining experimental work with computational studies to gain a deeper understanding of how these materials function. "Our approach involves using macroscopic techniques for fully characterising new materials," he says. "Then, if we find sufficiently interesting properties, we use local probe techniques to provide more details."

Dr João Pedro Esteves de Araújo

Dr Armandina Lopes

The group's work has covered materials with a broad variety of physical properties, from high-temperature superconductors to colossal magnetoresistance oxides. More recently, they have been looking at room temperature magnetoelectric compounds, in which the magnetic and electric properties of the material are coupled. It is thought that materials known as perovskites may represent good candidates for creating such compounds.

Perovskites are materials with a specific crystal structure and the chemical formula ABX_3, where 'A' and 'B' represent cations and X is an anion that bonds to both. Many different elements can be combined to form perovskite structures and, using this compositional flexibility, scientists can design perovskite crystals to have a wide variety of physical, optical, and electrical characteristics.

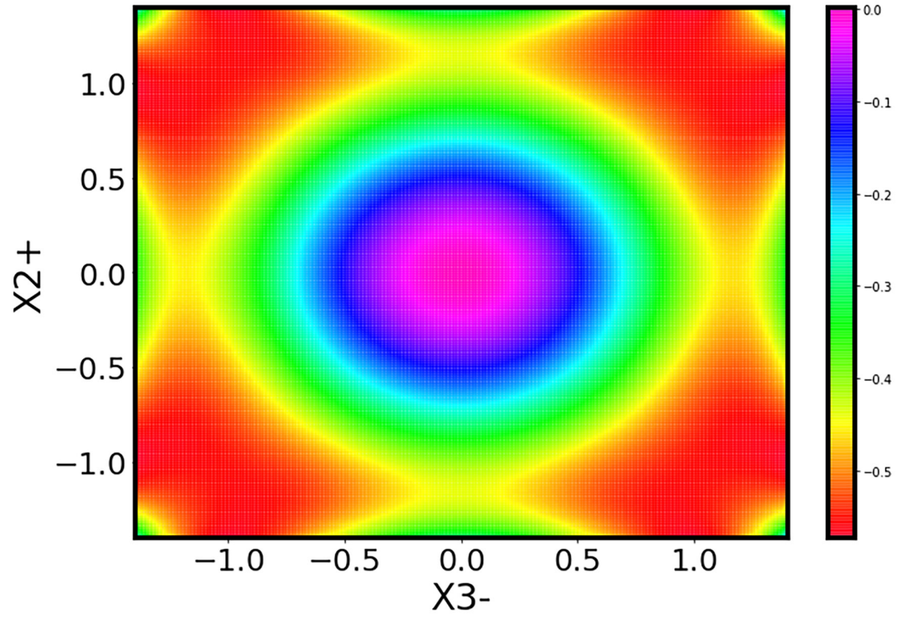
Although the structures of perovskites are simple, they can be used as building blocks to create more complex structures that have several interesting properties. These properties can be tweaked and refined by introducing instabilities in areas known as oxygen octahedra. Dr Armandina Lopes, a senior researcher and colleague of Araújo at the University of Porto, explains how a recent PRACE project has helped them investigate these materials. "Using simulations, we can play around with the rotation and tilt of these octahedra to enhance the ferroelectric and magnetic properties of the materials. We can predict the properties of these proposed materials extremely accurately, providing us with insights that macroscopic techniques cannot."

Araújo's team has been carrying out this computational work as part of a larger project in which others have been synthesising the materials and characterising them using local probe techniques at CERN. "We realised that we needed much more computational power than was available in Portugal to match up with the experimental work being done," he says. "That is why we applied for this PRACE project, and it has really helped to bring our team together in terms of getting theoreticians, computer-oriented physicists and experimentalists to work towards a common goal."

Following a previous publication that described a new group of multiferroic materials developed in this way called hybrid improper ferroelectrics, Araújo and his team have been able to study them further, particularly looking at a property known as negative thermal expansion. Typically, materials increase in volume when their temperature increases, but these materials do the exact opposite. As well as this being interesting in its own right, there are a number of potential applications for materials with this property, for example high-precision optical and microelectronic devices. This PRACE project has allowed the team to understand the mechanism via which it occurs in natural layered perovskites.

More information
http://www.ifimup.up.pt

HPC Resources awarded by PRACE
These projects were awarded a total of 25 700 000 core hours on Marconi100, hosted by CINECA, Italy.

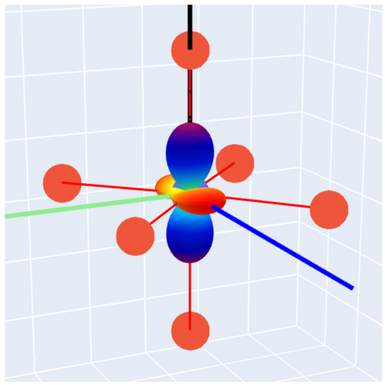


Energy barrier according to polarization switching via the X_{2+} or X_{3-} irreducible representations of the $I4/mmm$ space group. The center (large energy area) represents the structure with no rotation and no tilt applied, i.e., the $I4/mmm$ space group. The red corners (low energy area) represent the four possible structural domains of the phase transition to the $A2_1am$ space group.

One of the properties that the team were able to measure at CERN in the hybrid improper ferroelectric materials is what is known as the electrical field gradient. They have now had a paper published which made the cover of Journal of Materials Chemistry C that looks at the relation between electrical field gradient and the structures of these materials.

As many scientists will confess, research often creates more questions than it answers. While using what is known as local probe techniques to study their materials at the ISOLDE facility at CERN, the team began questioning whether the probe itself could become part of the material, as Araújo explains: "We were using an isotope called cadmium-111m as our measurement probe, when we started imagining ways in which this isotope could be used as an element in new materials. We are now working on simulations to explore the potential of cadmium."

The group has now won a further allocation of computing time from PRACE in order to continue their work. While the previous work was done on the Marconi100 machine, Araújo was advised to apply to a different machine – Joliot-Curie – for this next stage. "When you submit a proposal with PRACE, it undergoes a rigorous process of technical and scientific review," he says. "Our referees saw that we were looking to use genetic algorithms to generate potential new structures that we could then test, and pointed us towards tools that could do this in an integrated way. However, these tools were much better suited to the Joliot-Curie architecture, so we were glad to receive this advice in the process of applying."



Electric field gradient surface of Mn at the high-temperature centrosymmetric structure with space group $I4/mmm$. Green, blue, and black lines represent Vxx, Vyy and Vzz directions, respectively. Red spheres represent oxygen atoms.

Studying the structures of Cooper pairs

Unconventional superconductivity

Recent theoretical developments by **Professor Mark van Schilfgaarde** of King's College London have led to the creation of a high-fidelity method for describing the electronic structure of unconventional superconductors without over-reliance on models. His success in using it on high-performance computers marks a first step towards a systematic theory of unconventional superconductivity that would provide a powerful tool in the search for the holy grail of room-temperature superconductors

Superconductors have long tantalised the world with their potential for powering futuristic technologies such as super-fast levitating trains and lossless electrical wiring. Their ability to offer no resistance to electrical current and expel magnetic fields relies on bound pairs of electrons called Cooper pairs, and it is the tendency for all Cooper pairs in superconductors to "condense" into the same ground quantum state that is responsible for their peculiar properties. However, researchers have yet to discover any material that displays superconductivity at room temperature – the key to unlocking their technological potential.

In conventional superconductors, Cooper pairs are formed when negatively charged electrons – normally repulsed by each other – are bound together via their interaction with the positively charged lattice of the material. This is known as an electron-phonon interaction, the phonon being the quantum mechanical description of a lattice vibration.

However, in the late 1980s, another class of superconductors called unconventional superconductors was discovered in which the Cooper pairs were not bound via this mechanism, instead showing more complicated structures that are thought to be related to fluctuations in the intrinsic angular momentum – or spin – of the electrons.

Professor Mark van Schilfgaarde of King's College London is an expert in the theory of electronic structure, the key to understanding properties of materials at their most fundamental level. He is particularly known for his work in Quasiparticle Self-Consistent GW theory (QSGW), a new formulation of one of the most advanced approaches to electronic structure – the GW approximation. QSGW dramatically improves the quality of GW and makes it suitable for studying a number of interesting materials.

Professor Mark van Schlfgaarde

A recent development of QSGW aimed to extend the theory to treat strongly correlated systems such as unconventional superconductors by combining it with dynamical mean-field theory (DMFT). DMFT is a non-perturbative theory that provides information about the short-range correlations between electrons that GW cannot. "As long as you are working with a strongly correlated system where all the interesting things happen within a few degrees of freedom – as is the case with unconventional superconductors like iron selenide and YBCO – DMFT is much more tractable than GW," says van Schilfgaarde.

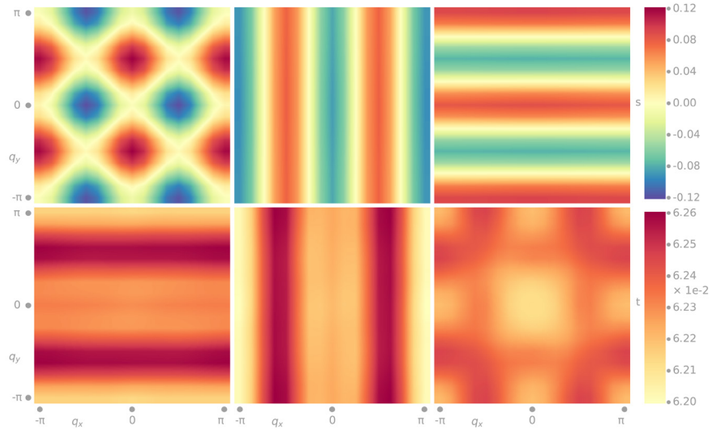
Around twenty years ago, researchers began using DMFT in conjunction with density functional theory to study materials, but by using GW instead of density functional theory, van Schilfgaarde has created a high-fidelity theory that can accurately describe unconventional superconductors and provide information about the structure of their Cooper pairs.

DMFT provides a way of partitioning the study of unconventional superconductors into two parts – a strongly correlated part and a weakly correlated part. The whole system is first calculated using QSGW, after which the strongly correlated sub-space is calculated using DMFT and embedded into the original calculation. The influence of this sub-space on the rest of the system is then calculated to make it self-consistent. This process is then repeated over and over until a quantity known as the Green's function stops changing.

More information
https://www.kcl.ac.uk/people/mark-van-schilfgaarde
https://www.questaal.org/

https://www.nature.com/articles/s42005-019-0254-1

HPC Resources awarded by PRACE
This project was awarded 40 000 000 core hours on Joliot-Curie – Rome, hosted by GENCI at CEA, France.



The superconducting pairing gap symmetries for εx=0 are shown in the (100)-(010) plane of the reciprocal lattice; eigenfunctions corresponding to first three eigenvalues in singlet (s) symmetries are in the top panel and triplets (t) are in the lower panel

"Our theoretical developments have helped us make a lot of progress," says van Schilfgaarde. "We are a long way from solving everything, but we can do things that we could not do before, like predicting the superconducting critical temperature and examining the way in which the superconducting state competes with other states like ferromagnetism."

This theory has for the first time provided a method for studying the structure of Cooper pairs in unconventional superconductors without relying on density functional theory or on models. "A big problem in the field of superconductivity research is that it is so complicated that it almost entirely relies on models," explains van Schilfgaarde. "This is not to denigrate the work of those who create these models – these people are brilliant physicists who have created intricate and ingenious theories for explaining superconductivity. However, the models all rely on assumptions that we have no basis for knowing whether they are correct or not, which has led to a lot of confusion in the literature and a lack of consensus about the mechanisms behind superconductivity."

His method has now been used with great success to study a number of unconventional superconductors, using the power of high-performance computers provided by PRACE to solve the complex DMFT equations. One example involved the investigation of the critical temperature of iron selenide. In bulk, the critical temperature of this material is 8.5K, but recent experiments showed that if a monolayer of it was deposited on top of strontium-titanate, the critical temperature jumped to around 100K. The reason for this jump in critical temperature was originally thought to be due to assistance from electron-phonon interactions, but van Schilfgaarde's calculations indicate otherwise.

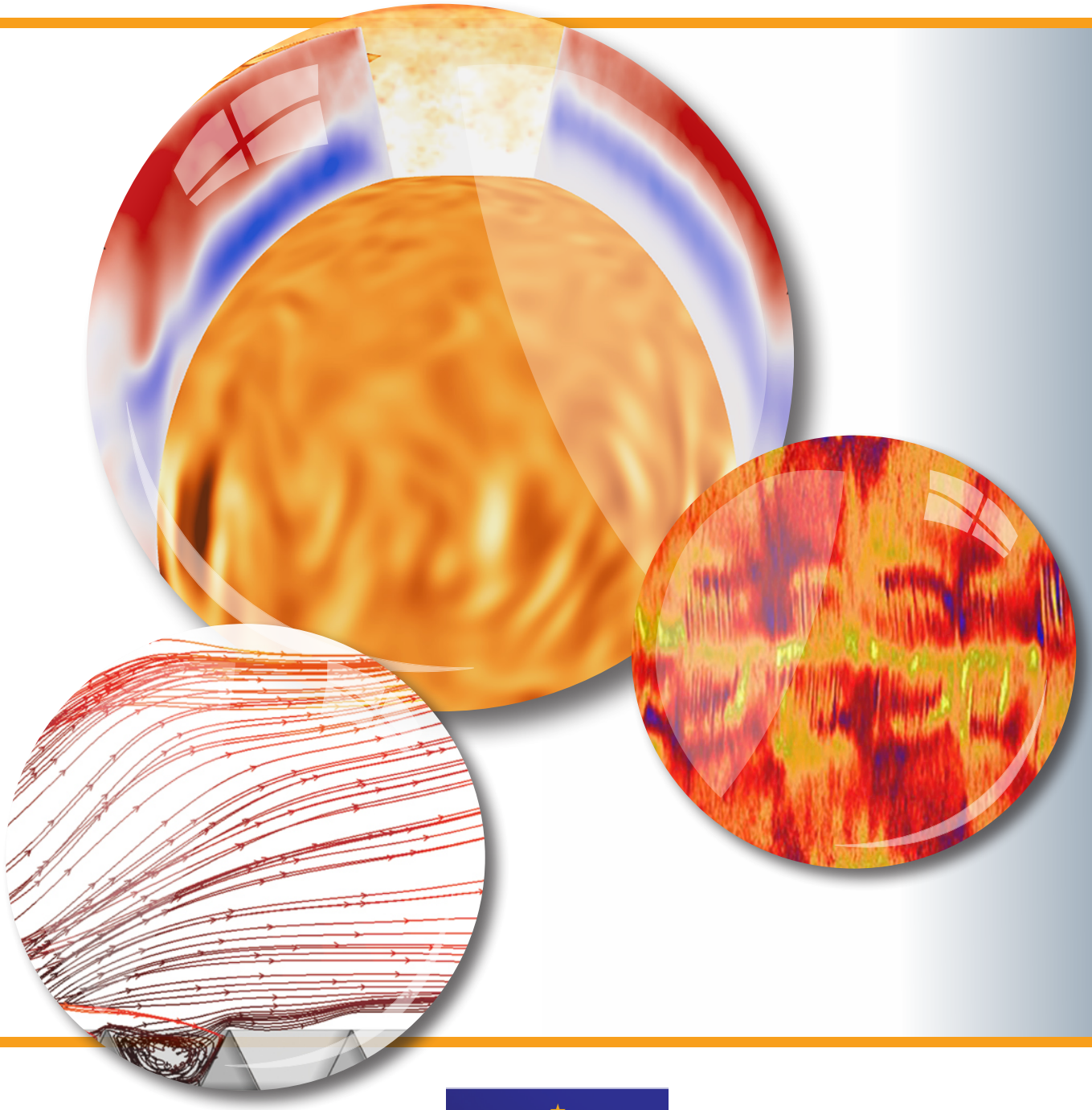
"Our calculations showed that the real reason for this jump in critical temperature is due to a small change in what is known by modellers as the Hubbard Hamiltonian parameter, which causes a massive change in the incoherence of the electrons and thus the critical temperature. We showed in our simulations that if you tweaked this parameter for the material in bulk, the same increase in critical temperature was achieved."

Strontium ruthenate is another material that has been investigated by van Schilfgaarde. Until a few years ago, it was considered a prime candidate for being a spin triplet superconductor. Discovering such a material is of great interest as it would allow for the creation of Majorana fermions, long-sought exotic particles that are their own antiparticles, and which many think could act as stable qubits that would revolutionise quantum computing.

However, recent experiments have cast doubt on its credentials as a spin triplet superconductor, showing that the temperature of the probe used in the original study may have contaminated the results. "We used our theory to look at strontium ruthenate and showed that three spin triplet states do exists within it, but they are in competition with three spin singlet states," says van Schilfgaarde. "The spin singlet emerges as being a little stronger, which indicates strontium ruthenate is not the spin triplet superconductor it was widely believed to be."

The team from King's College London have now studied enough systems to be fairly confident that their theory is capable of describing many kinds of unconventional superconductors. The method represents a first step towards developing a systematic theory of unconventional superconductivity, which will provide a powerful tool in the search for the holy grail of room-temperature superconductors.

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE



The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 823767

www.prace-ri.eu