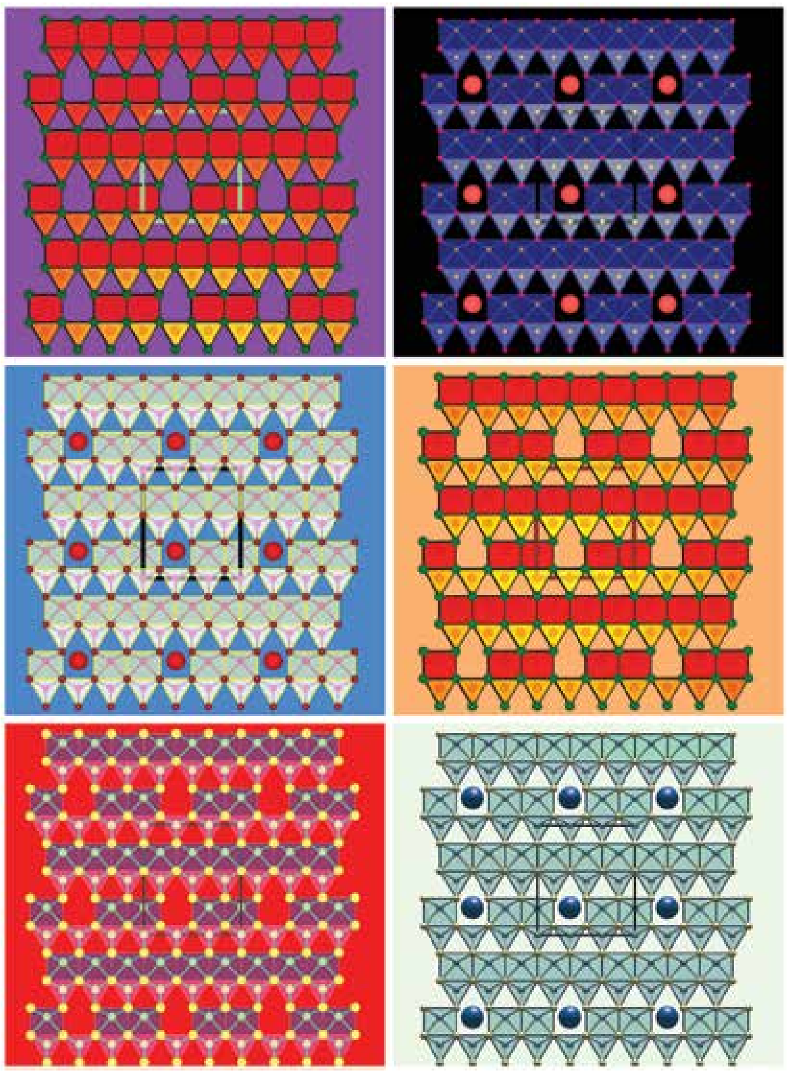
2017



Vacancies in a Weyl semimetal under different conditions

Dr John Buckeridge, Department of Chemistry,
University College London

These images show the results of calculations performed to determine the minimum energy atomic configuration of TaAs, a semimetal in which the rare, exotic particle known as the Weyl fermion was finally discovered last year, after over eighty years of searching. These particles arise due to favourable electronic energy states in the perfect, pristine material and may be of use in quantum computing applications. Here the system is missing one Ta atom, which affects the electronic structure of the material and hence the presence of the Weyl fermions.

January

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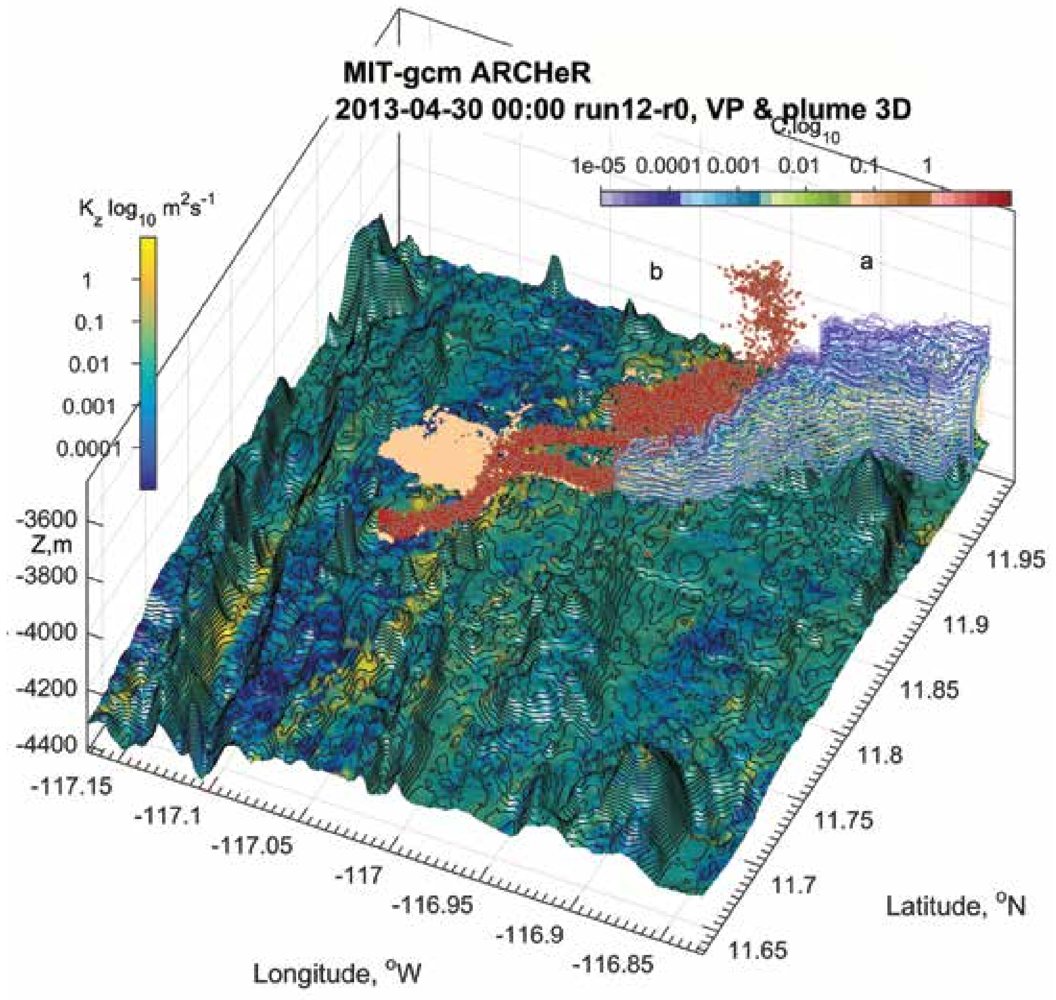

Numerical experiments with 3D plume dispersal over a deep-sea mining site

Dr. Dmitry Aleynik, Scottish Association for Marine Science

Harvesting of ferro-manganese nodules deep below the surface in the Central Tropical Pacific will generate plumes of suspended sediment with inevitable ecologically harmful long-lasting impact to the fragile, diverse, unique and largest abyssal benthic community on earth. Alongside concessions licenses, which have tripled in the past 6 years, a tool to assist spatial preservation planning is urgently required. To estimate plumes advection, the flow field was computed on ARCHER using an MIT-gcm general circulation model, forced by tides and the observed (in spring 2013) currents at the proposed mining site in the eastern Clarion-Clipperton Zone. The figure shows a neutrally buoyant tracer spreading over a 3D bathymetry with colours indicating the concentration of dissolved matter (a) and overlaid with vertical mixing strength (Kz) after 19 days. Particulate matter plume contains half a million individual particles either suspended in a water (magenta) or settled on the seabed (pale) and charted on the same date (b).

February

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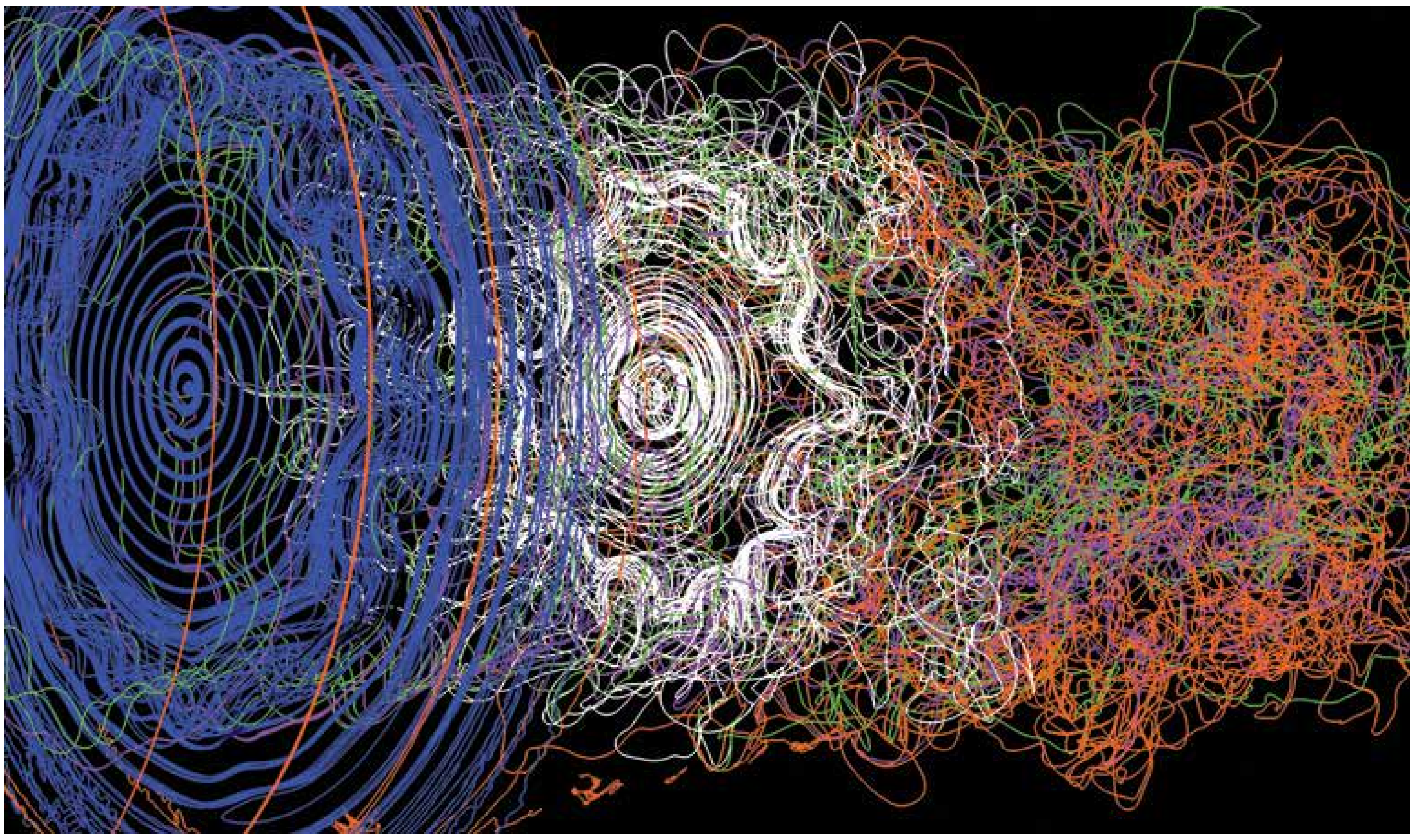

Vortical lines evolving in a turbulent jet flow from a round nozzle

Mr Vassilis Ioannou, Aeronautics, Imperial College London

This image shows the evolution of a turbulent high-speed air jet ejected from a round nozzle in slow-moving air. The flow near the nozzle-exit is based on large-scale annular structures whereas the flow further downstream is highly turbulent with structures over a wide range of scales. The turbulent jet is a canonical flow representative of many practical applications such as, e.g., propulsion jets of aircraft engines, hazardous toxic gases released from smokestacks, wastewater discharge from pipes into rivers. Our aim is to manipulate the flow structures at the exit of the nozzle in order to achieve noise mitigation and mixing enhancement. The data was produced by a high-fidelity simulation for which the equations describing the fluid motions were solved with the open-source flow solver Incompact3d (www.incompact3d.com). The simulation was performed on ARCHER in a domain using more than 800 million nodes on 8,192 cores.

March

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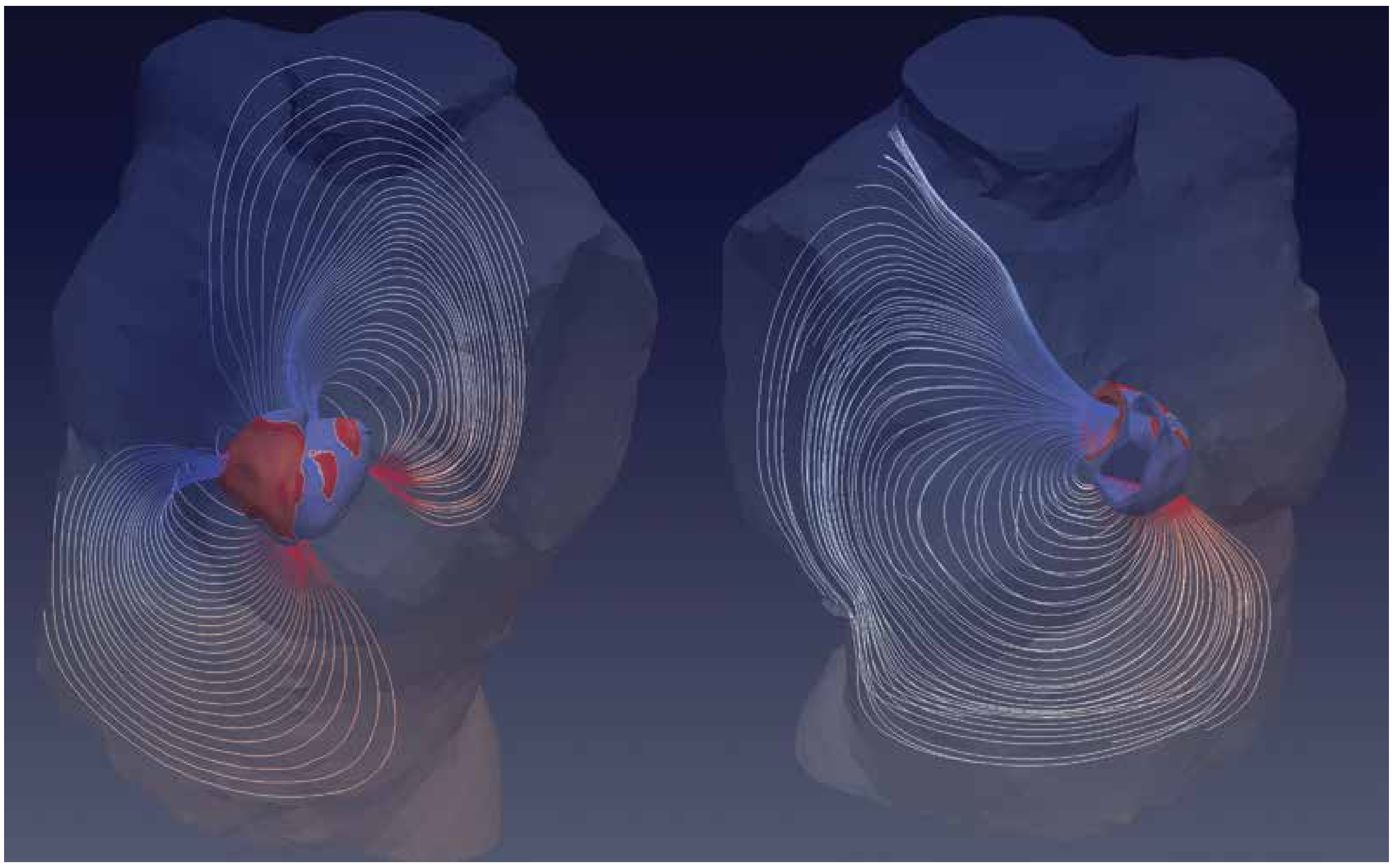

Electric field generated by the heart in the human body at the beginning of a heartbeat in healthy (left) and diseased (right) conditions

Dr Alfonso Bueno Orovio, Department of Computer Science, The University of Oxford

The figure shows the electric field generated by the heart in the human body during the initiation of a heartbeat. This is shown for a healthy person (left) and for a person with the diseased condition known as right bundle branch block (right), where your right ventricle is not able to activate properly. In the heart, the red colour indicates the areas that have been electrically activated, while those in blue are areas yet to be excited. In the body, the streamlines show the electric field produced by such an electrical activity, coloured by electric voltage potential. This can be measured for diagnosis in the clinic in the form of an electrocardiogram. The use of ARCHER has allowed the investigation of multiple disease conditions in the human heart, to augment information that has been obtained from these signals for a better diagnosis of patients, and to improve their tailoring of therapy.

April

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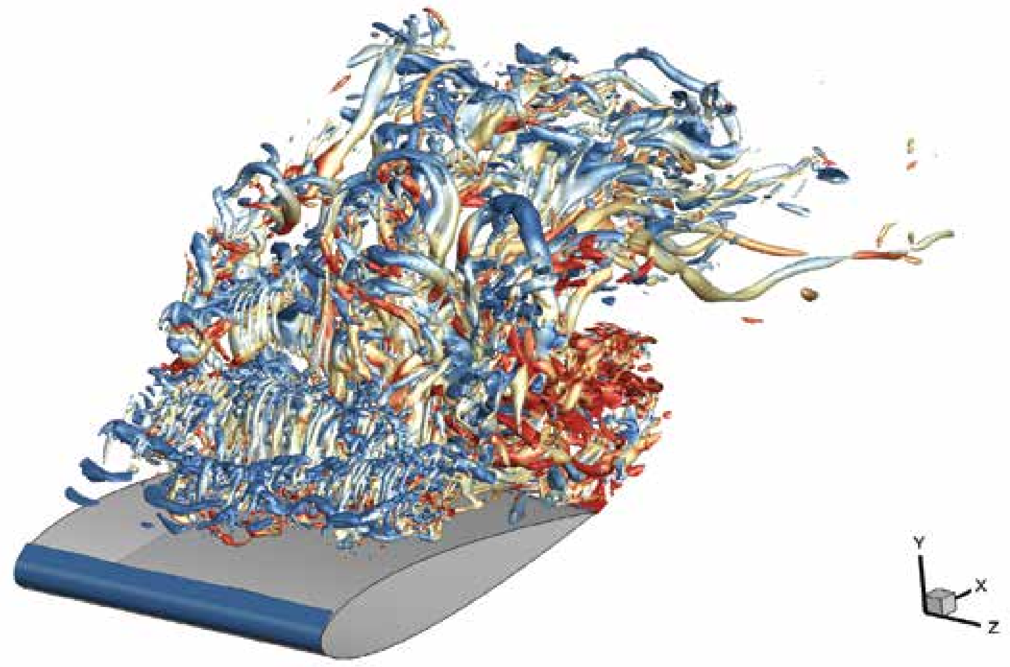

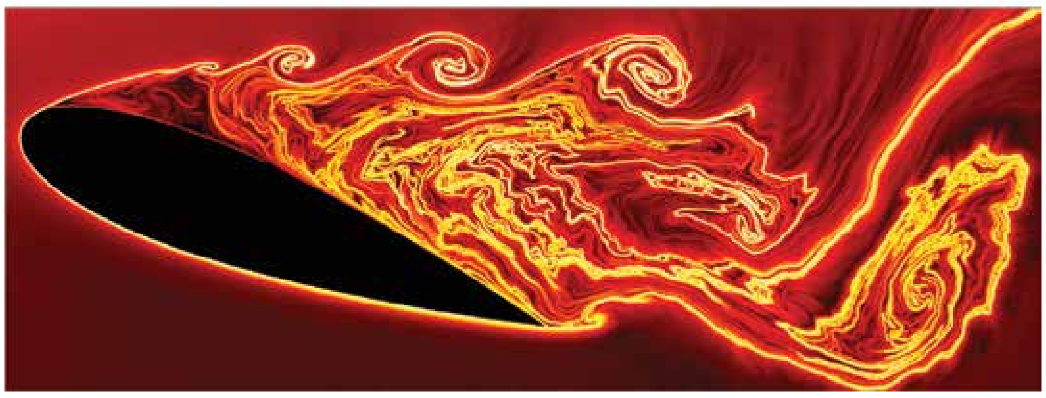

Three dimensional, unsteady, flows around an aircraft wing in various flight conditions

Dr. Marco Rosti, Dr Mohammad Omidyeganeh and Prof. Alfredo Pinelli, Dept. of Mechanical Engineering and Aeronautics, City University of London

We have studied the three dimensional, unsteady, flows around a wing in various flight conditions, mimicking those experienced during take-off and landing or the influence of a wind gust. With the aid of numerical simulations, as an alternative to experiments in a wind tunnel, we were able to develop new wing designs that can enhance aerodynamic performance at no extra cost. These can improve an aircraft's manoeuvrability, increase the amount of weight it can carry, or reduce the fuel consumed – all of which may contribute to reductions in greenhouse gases. The picture shows the isosurfaces of the Q-criterion (top) and the Lagrangian Coherent structures (bottom) of an aerofoil at 20° of incidence at Re=20000.

May

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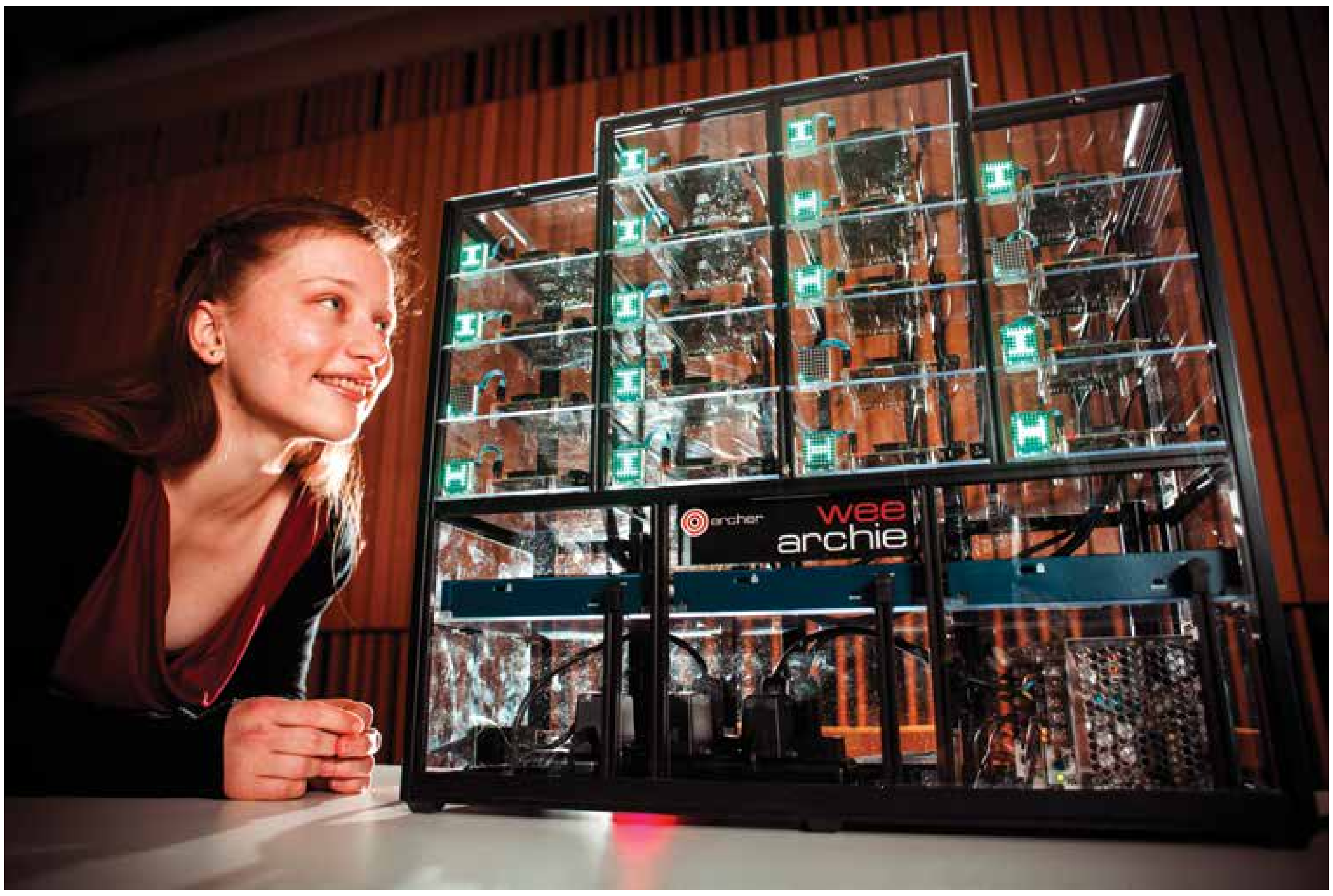

Wee Archie – The suitcase-sized supercomputer
Dr. Lorna Smith, EPCC, The University of Edinburgh

Wee Archie is a suitcase-sized supercomputer, designed to let school children try their hand at computing and learn about the benefits of supercomputing. The system has been created to be representative of the system design in massively parallel architectures. There are 18 Raspberry Pi's, each acting as a multi-core node providing a total of 72 cores and 144GB of RAM, a network switch, a power supply unit (PSU) and Ethernet cables. Each Raspberry Pi has an LED display that lights up when in use, providing a visual display that helps demonstrate how multiple processors work in parallel to solve complex tasks. We have a suite of demos for Wee Archie. These demos highlight real science from the ARCHER system and show the benefits of ARCHER in a fun and accessible manner.

Wee Archie was designed and built through a collaboration between EPCC and Edinburgh University's science outreach group, FUSION.

June

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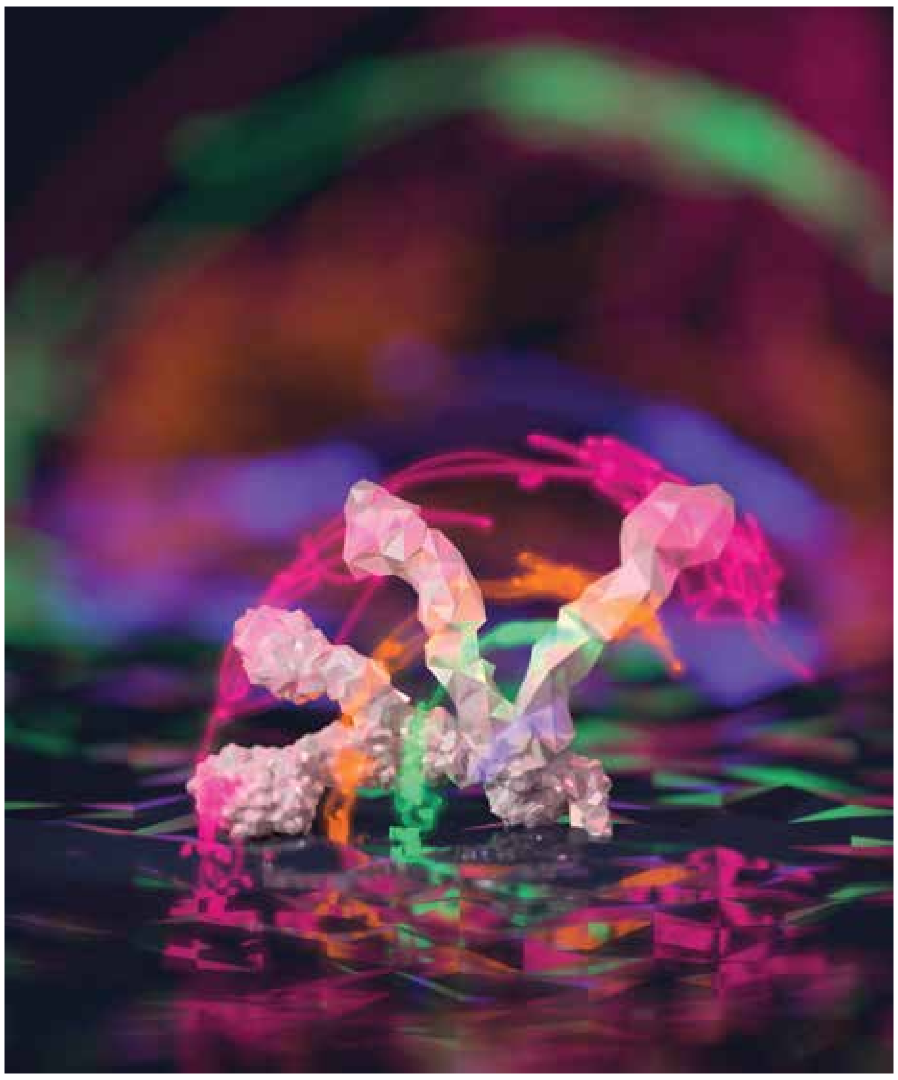

Model of EphA2 ectodomain at the membrane

Dr Matthieu Chavent and Mr Tom Newport, SBCB, Biochemistry Department, The University of Oxford

EphA2 is a Receptor Tyrosine Kinase belonging to the Eph family. Eph receptors and their ephrin ligands are key regulators of cell-cell signaling and cells migration. These receptors share a similar molecular architecture, with an extracellular domain (the ectodomain), an α-helical trans membrane domain, and a cytoplasmic signalling region. It is thus important to understand how the ectodomain of EphA2 is oriented at the membrane as this will provide insights on the modulation of the activity of this receptor and how it can transfer signals across the cell membrane. We have modelled the interaction of the ectodomain of the EphA2 receptor with a lipid bilayer (here represented by triangles or cubes). Multi-scale simulations based on this model reveal the flexibility of the ectodomain. The image illustrates the simulated dynamics of the ectodomain (shown as glowing lines) as well as different conformations that highlight the possible movement of this receptor relative to the membrane surface.

July

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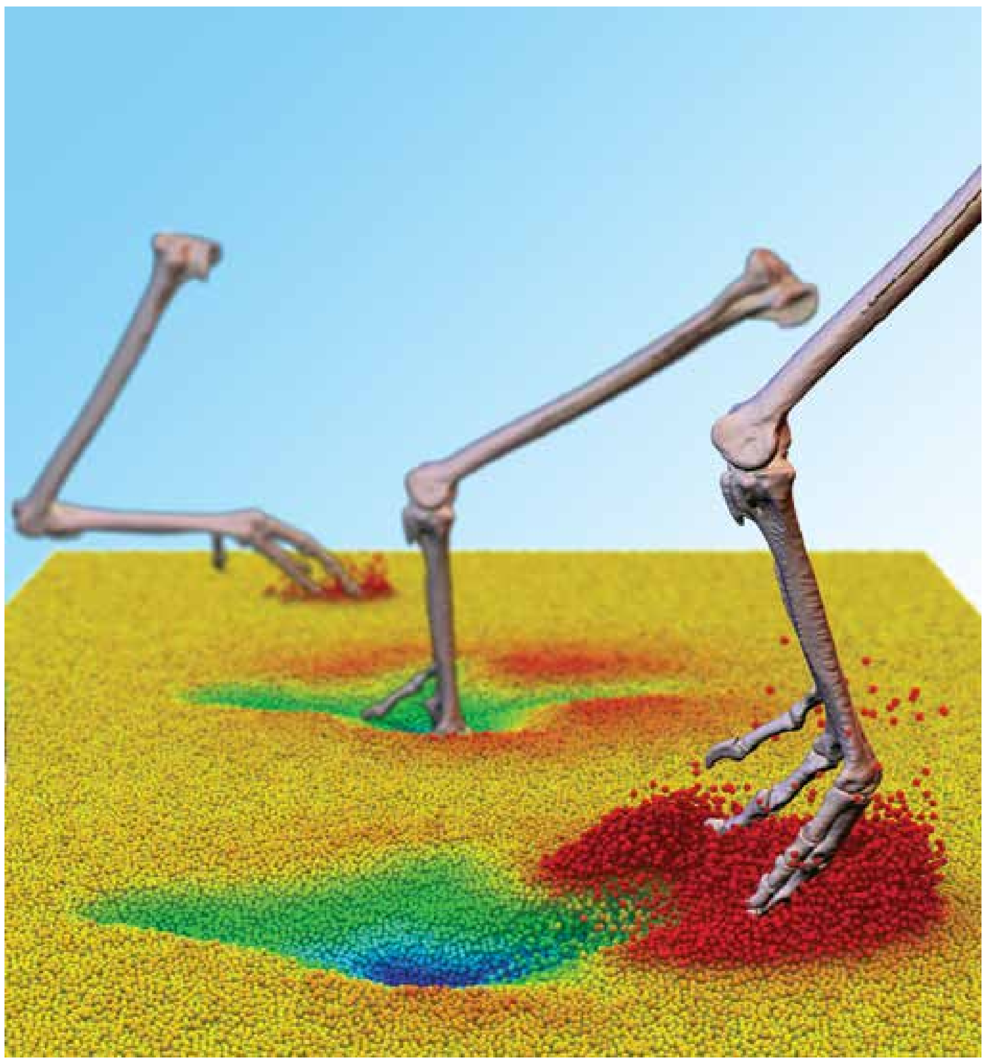
COMPETITION WINNING ENTRY



The birth of a footprint

Dr Peter Falkingham, Natural Sciences & Psychology,
Liverpool John Moores University

This image is of three stages of footprint formation, simulated by combining bi-planar X-ray data of a guineafowl walking over a sand-like substrate with a Discrete Element simulation of the substrate. X-ray Reconstruction of Moving Morphology (XROMM) was used to capture the motions of the leg and foot in a living animal. LIGGGHTS was then used to model the substrate, simulating grains of 1 mm diameter. Poppy seeds were used as the substrate as they behave like dry sand but are less dense, allowing X-rays to pass through.

This work has allowed us to link features of footprints - both at and below the surface - with motions of the foot, and is now being applied to understanding footprints made by long extinct dinosaurs.

August

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A "Pac-enzyme" in action: thermodynamics analysis of domain motion

Dr. Danilo Roccatano, School of Maths and Physics,
The University of Lincoln

Our pac-enzyme, Citrate Synthase (CS) is an enzyme localized in the mitochondria of our cells where it plays an important role in the aerobic respiration cycle by transforming oxaloacetate molecules (on the right side of the picture) in citrate (on the top left side) with the assistance of the acetyl-coenzyme A (CoA) molecule. As the pac-man in the famous computer game, this Pac-enzyme diffuses along the space between the convolute cristae (the convoluted inner membrane) of the mitochondria "chomping" at encountered oxaloacetates. This activates the enzyme to bind the CoA (ghosts in the playground). For each captured CoA, a new citrate molecule is then produced (score). This complex mechanism requires large conformation changes of parts of the protein (domains) whose molecular details are not yet clarified. Using molecular dynamics simulations on the ARCHER supercomputer, we are studying this enzyme to garner novel insights on structural, dynamics and thermodynamics of its functional mechanisms.

September

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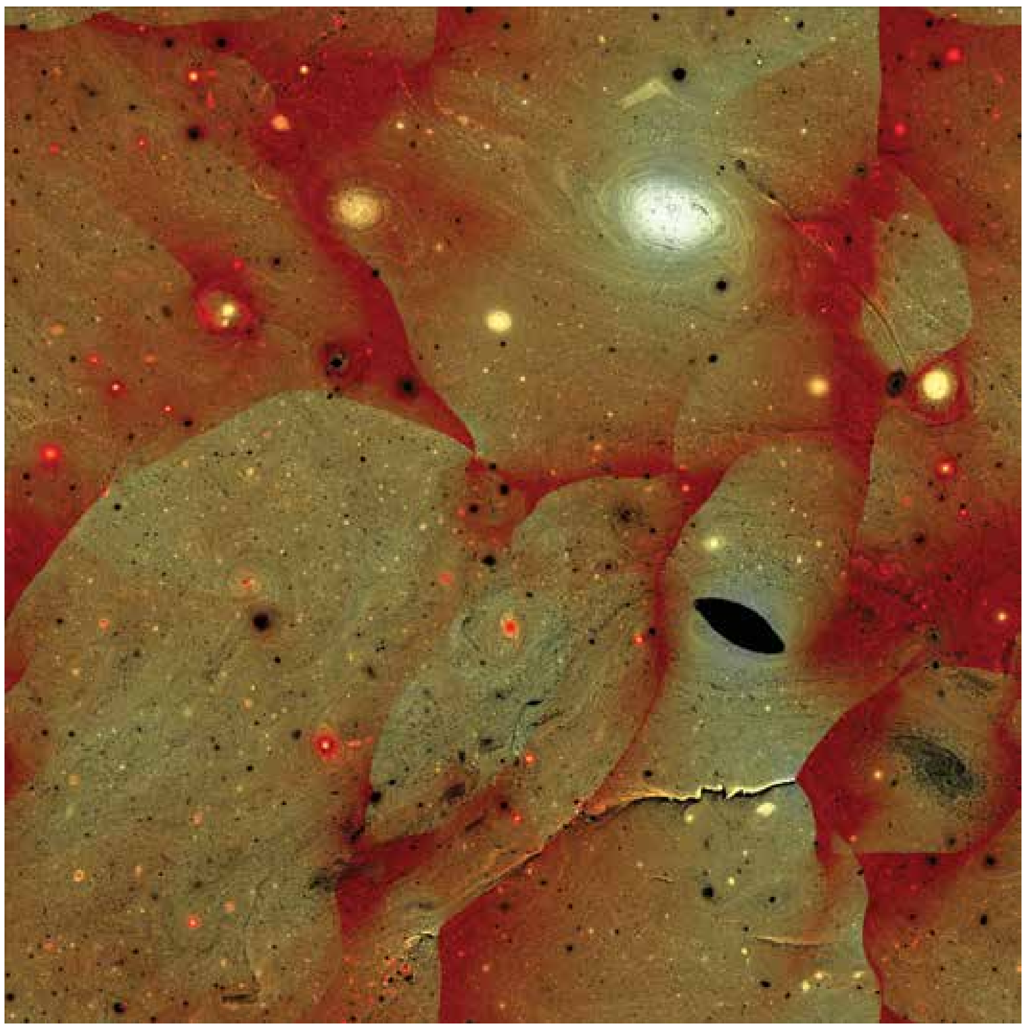

When turbulence meets a vanishing sound speed

Dr. Emile Touber, Mechanical Engineering,
Imperial College London

The picture is a snapshot of two-dimensional turbulence in the vicinity of the liquid-vapour critical point, where the speed of sound is nearly brought to a halt (red regions). Slowing down the speed of sound to such extremes gives birth to a wide range of non-linear wave phenomena not observed in ideal substances. These waves generate vast amounts of vortical structures (shown in black and white), which then significantly alter the way turbulence redistributes the kinetic energy across scales (the so-called energy cascade). These findings suggest that real-gas thermodynamics could offer a novel way of controlling turbulence (i.e. other than through boundary conditions or body forces), with possible applications in future energy production devices exploiting the properties of the liquid-vapour critical point. Capturing the kinetic energy redistribution process across scales requires significant computational resources such as ARCHER.

October

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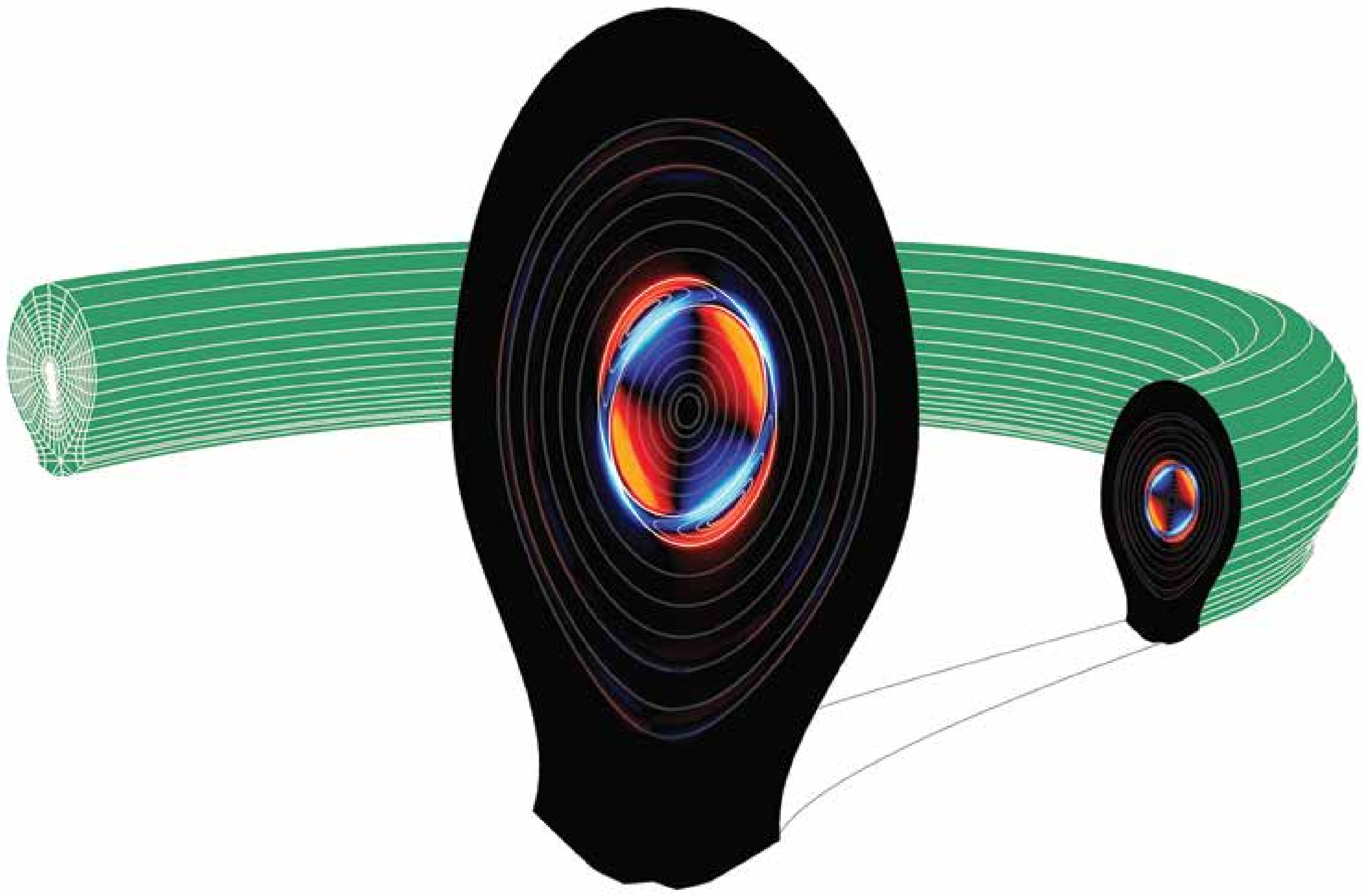

Harnessing the power of the Sun: Magnetic reconnection in a cross-section of a realistic tokamak simulated with the JOREK code

Dr Jane Pratt, M. Hoelzl and E. Westerhof, Astrophysics Group, The University of Exeter

Fusion is a process that heats the Sun and stars. If harnessed in the future, fusion could generate large amounts of carbon-free energy. A tokamak, a machine that uses a magnetic field to confine the hot ionized gas that makes up a plasma, has the potential to produce energy using fusion. In a tokamak, plasma resistivity causes magnetic field lines to reconnect, forming magnetic islands. When a magnetic island grows to a large size, it can result in fast escape of plasma from the machine.

This image shows a cross-section of a realistic tokamak configuration with a divertor, obtained as a snapshot from a simulation with JOREK, a nonlinear magnetohydrodynamics code. A large magnetic island is created by a perturbation of the current density which is indicated by the colours: negative current perturbations are displayed by blue colours, positive current perturbations are displayed by red colours. White lines have been plotted over the current perturbation to visualize the surfaces of constant magnetic flux. Outside of the magnetic island, these surfaces are nearly concentric. The size and position of the magnetic island is indicated by the surfaces of constant magnetic flux that form isolated pockets between the concentric circles.

November

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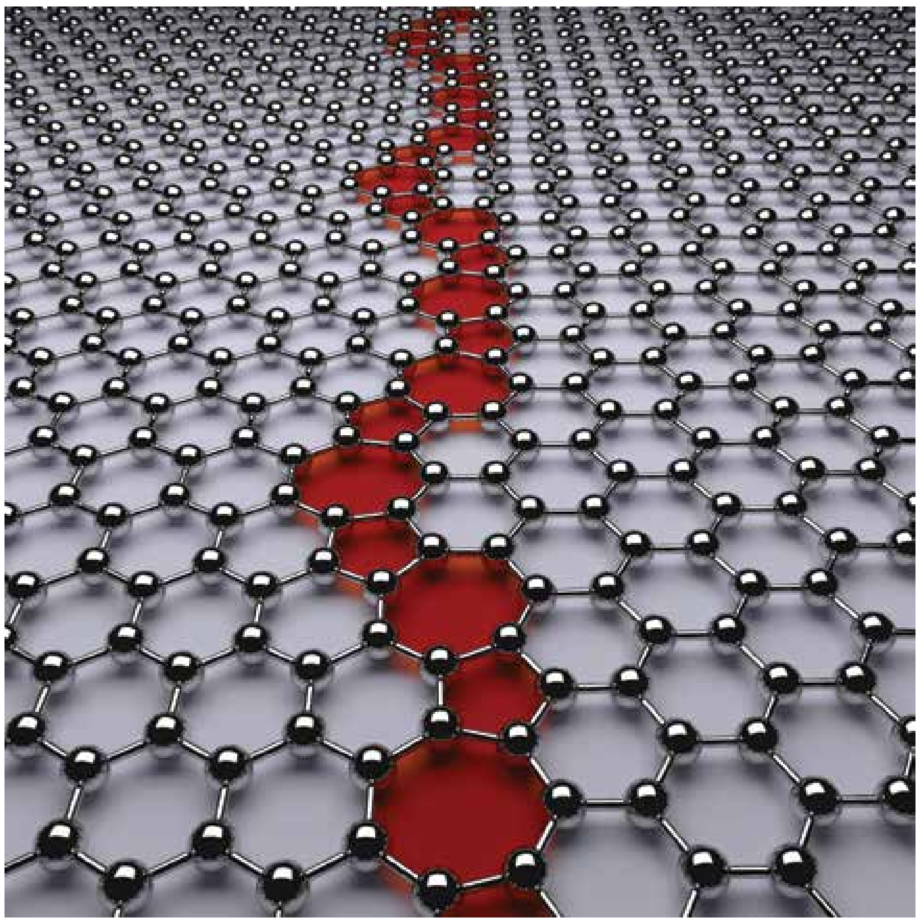

Graphene grain boundary

Dr. Georg Schusteritsch, Department of Materials Science and Metallurgy, The University of Cambridge

Graphene grain boundary structure between armchair and zigzag graphene regions - carbon atoms are shown as spheres. The red transparent region marks the interface between the two so-called grains, forming a continuous chain of pentagons and heptagons in the otherwise pristine graphene. The atomic structure was found using our crystal structure prediction code (AIRSS), implemented to employ the CASTEP code. Polycrystalline materials can today be routinely grown experimentally, but for many of these it is not easy to determine the atomic structures experimentally, making understanding their properties and the underlying physics that govern them a slow, difficult and often expensive task. Polycrystalline materials can today be routinely grown experimentally, but for many of these it is not easy to determine the atomic structures experimentally, making understanding their properties and the underlying physics that govern them a slow, difficult and often expensive task.

Crystal structure prediction in combination with the availability of the computational power from ARCHER, can be used to find the atomic structure of interfaces, and thus illustrate a future pathway towards computationally developing materials with specially designed interfaces. (DOI:https://doi.org/10.1103/PhysRevB.90.035424) [Image created using Blender 2.73].

December

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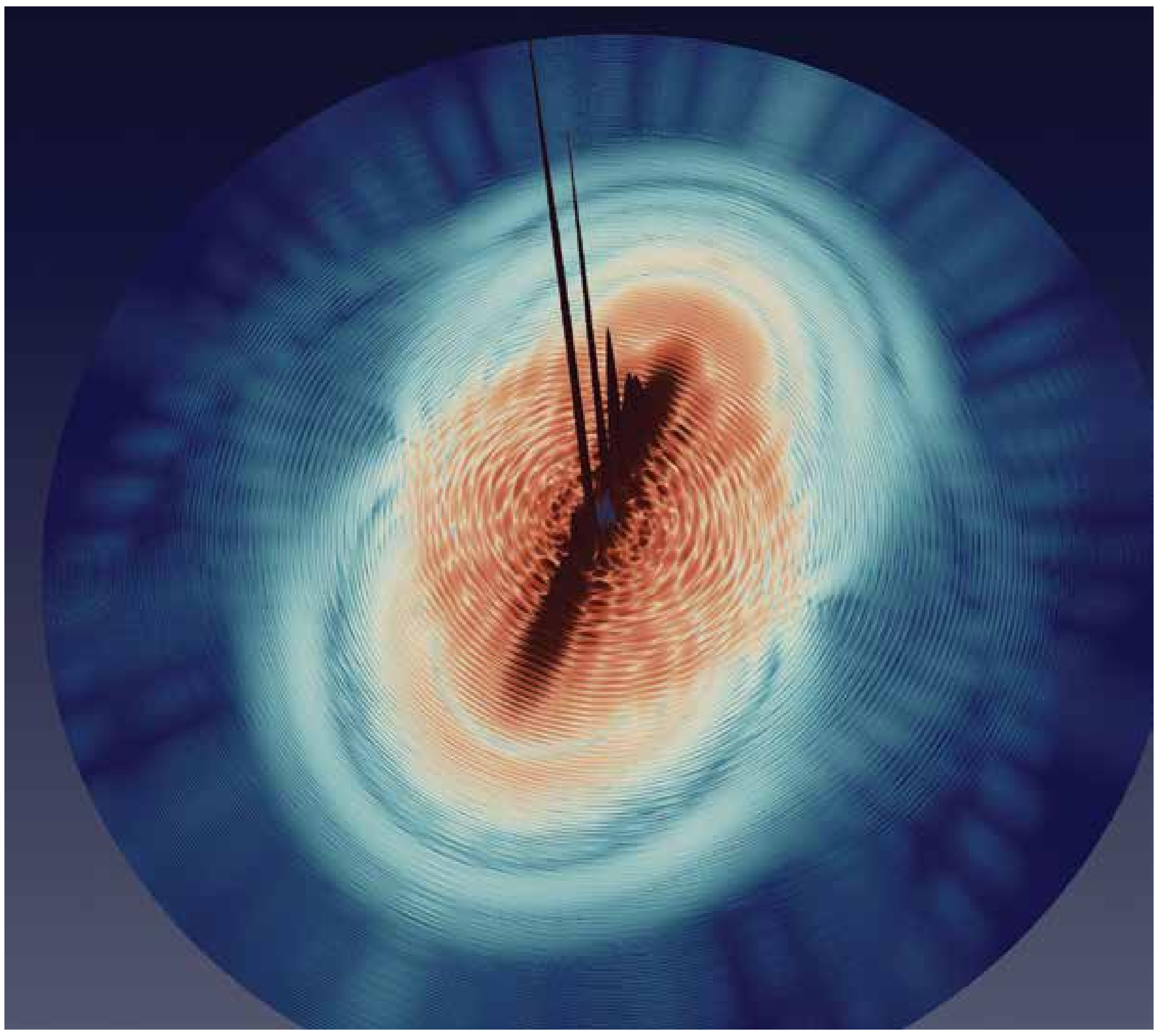


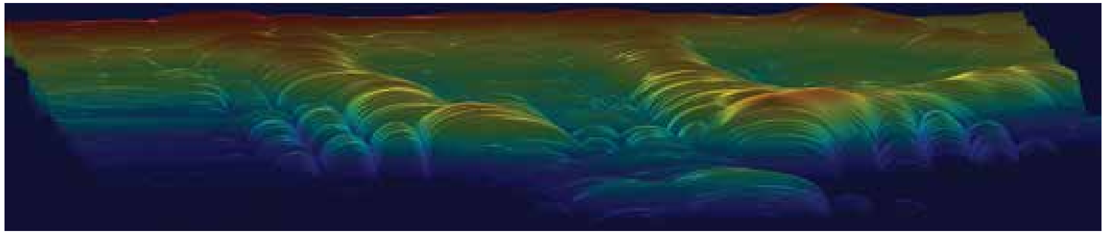
2D photo-electron momentum distribution after ionisation of a hydrogen molecular ion with an ultra-intense infrared laser pulse
Mr. Alejandro de la Calle, Atomistic Simulation Centre, School of Mathematics and Physics, Queen's University Belfast

Momentum distribution of an ionised electron from a hydrogen molecular ion after interaction with an ultra-intense infrared laser pulse. The circular structures with their centres along the central axis are due to rescattering of the electron against one of the two parent nucleus. The energy that the electron has gained from the field after ionisation allows for probing of the structure and dynamics of the parent system. For example, electron emission in a diatomic molecule as the hydrogen molecular ion presents a two-center interference, the same kind of interference present in a double-slit experiment. The data was obtained solving the time-dependent Schrödinger equation on a massively parallel calculation on the ARCHER supercomputer.

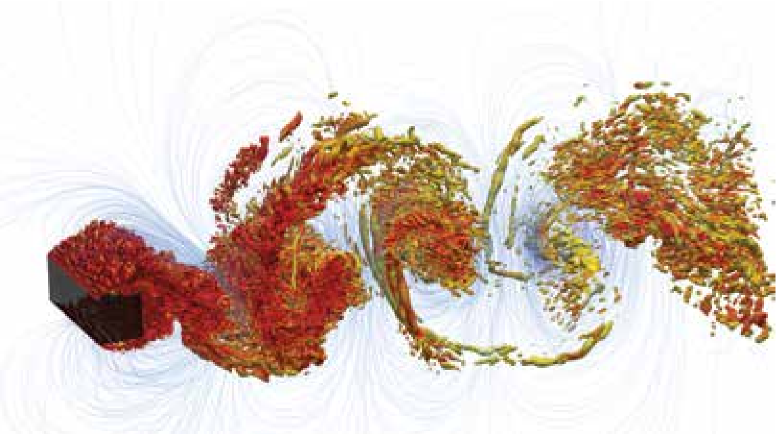
Notes

OTHER ENTRIES

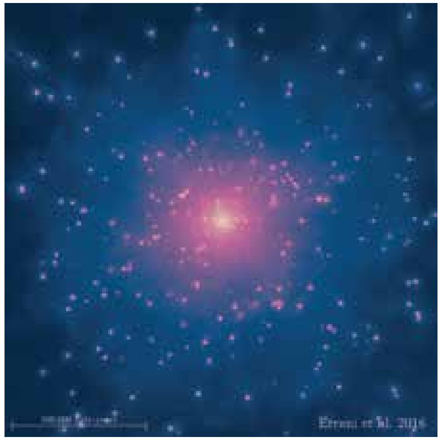
All the images in this calendar were submitted by ARCHER users as entries to the ARCHER Image Competition 2016. A gallery of all the images is available on the ARCHER website at **http://bit.ly/2016-Gallery**



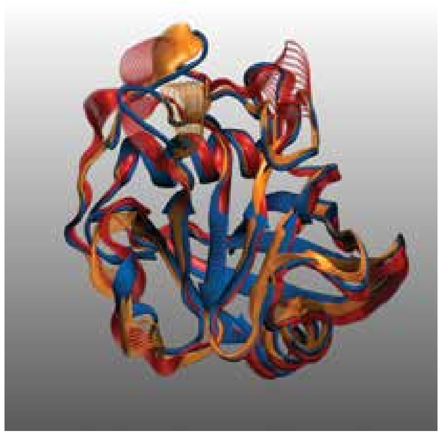
Stimulating competition between electrons with two colour light fields
Dr Andrew Brown, CTAMOP, Queen's University Belfast



Turbulent wake generated by a square prism
Mr. Felipe Alves Portela, Aeronautics, Imperial College London



Substructures in a Milky Way-like dark matter halo
Mr Raphael Errani, Institute for Astronomy, Royal Observatory, The University of Edinburgh



Eppur si muove. Computational simulations unravel hidden protein dynamics
Dr. Jordi Juárez-Jiménez, EaStChem School of Chemistry, The University of Edinburgh

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