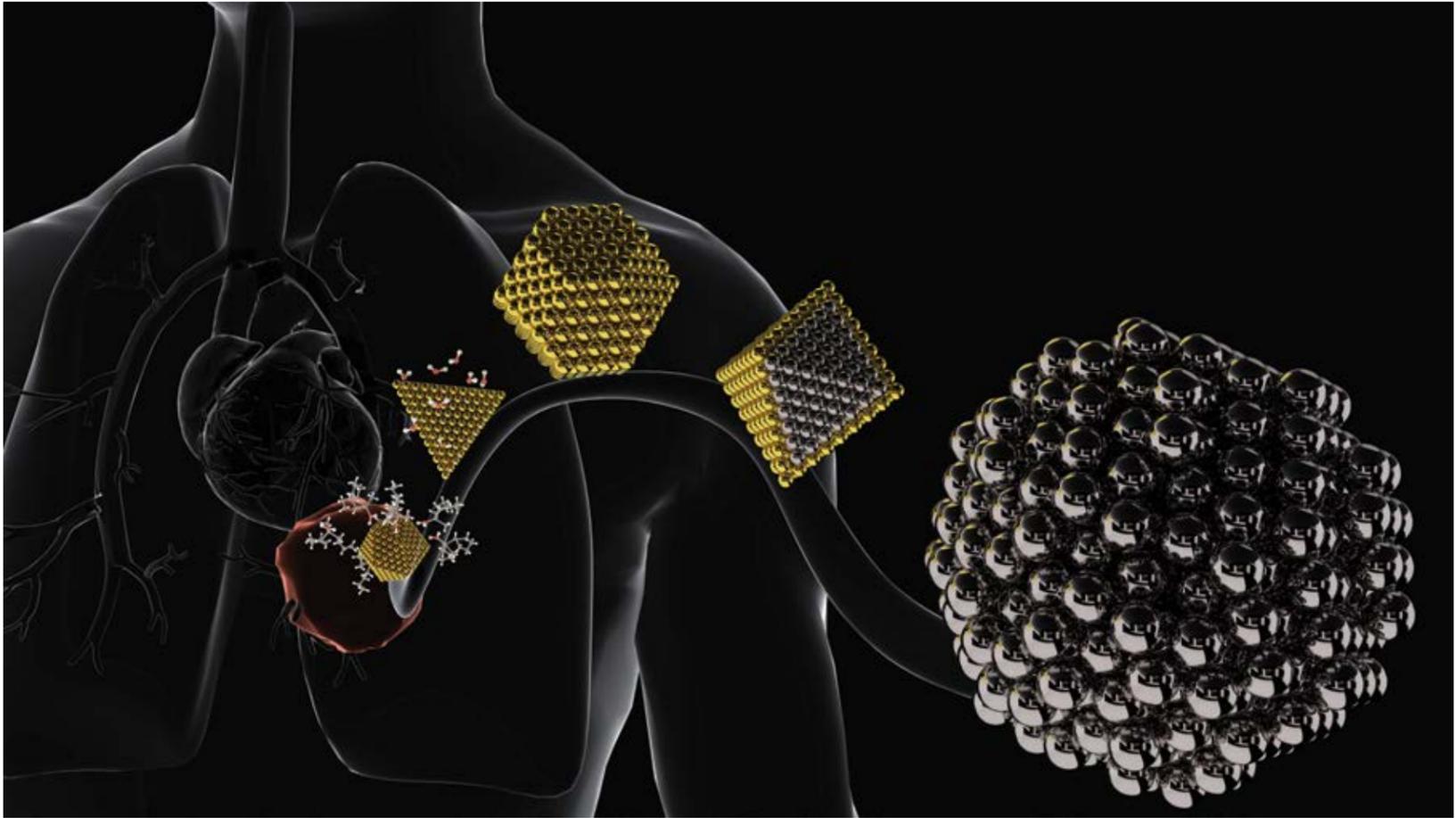




2019





A nanoparticle walks into a tumour (and other biomedical challenges): towards a morphology, size, and shape of perfect anti-cancer agents

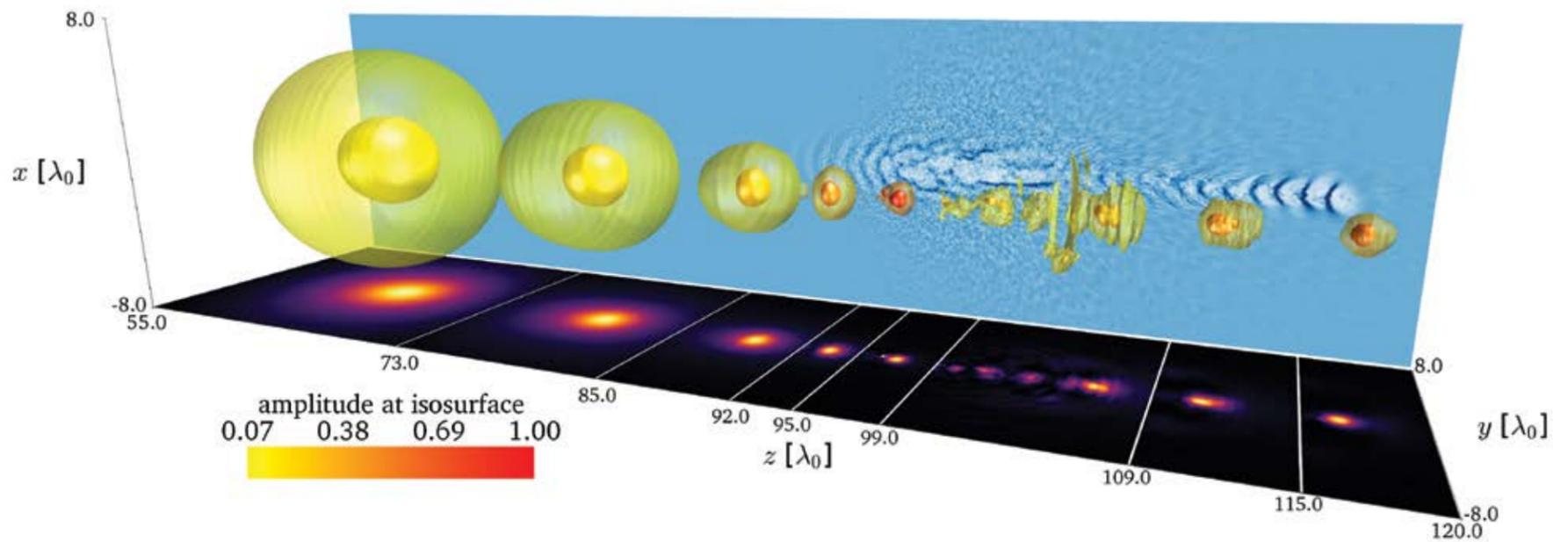
Barbara Farkas, School of Chemistry, Cardiff University

Nanotechnology has revolutionised cancer treatment in the last decade due to the unique properties packed in the nanosized features. Small sizes that are at the very limit of invisible, however, brought big challenges to experimentalists. The ability to investigate substances at the atomic level using supercomputers such as ARCHER has boosted both the analysis of compounds that were expected to perform well, and the search for new materials with outstanding properties for use in the biomedicine. This image shows the journey that starts with a cobalt nanoparticle, a nanoparticle made of highly magnetic but toxic metal and as such would never be considered a good candidate for cancer therapy, continues with the nanoparticle being modified with gold coating and functionalisation with biomolecules, to terminate with a multimodal nanocomposite that has both biocompatibility and power to fight the malignant disease. All of that thanks to the almighty engine of the ARCHER machine.

January



MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY	SUNDAY
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Spatiotemporally coupled laser pulse compression
 Thomas Wilson, University of Strathclyde,
 Physics Department

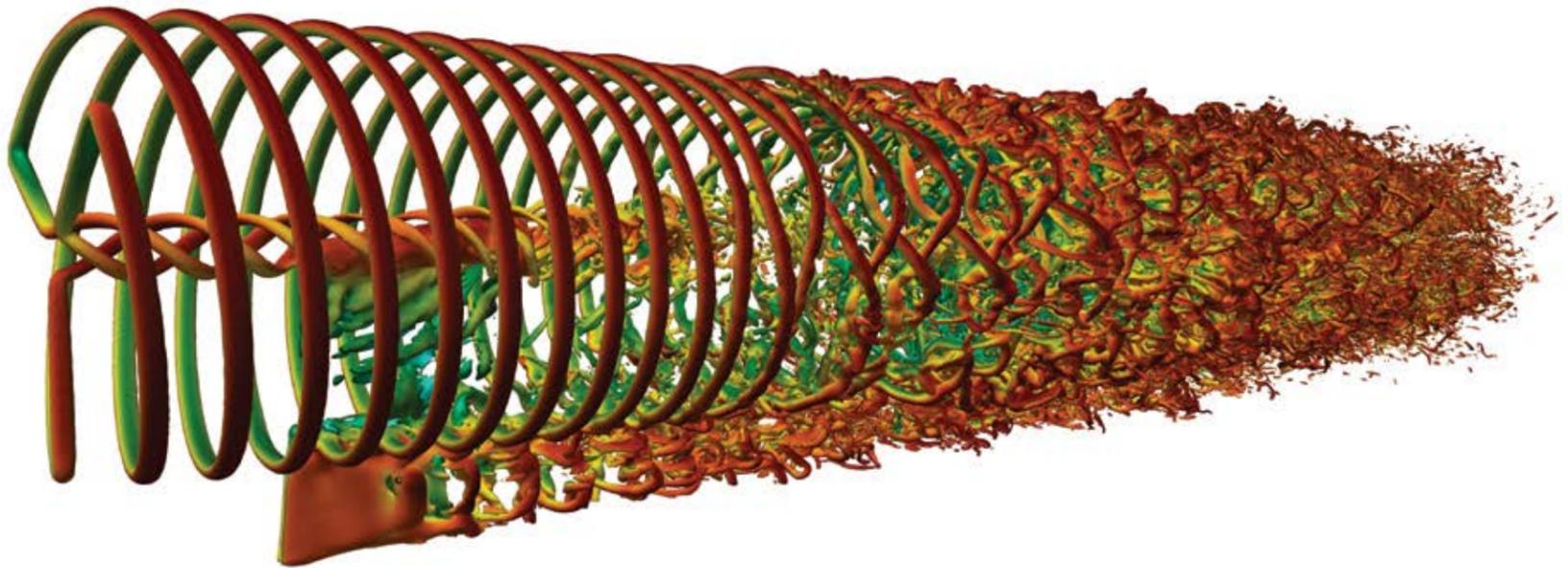
The manipulation of intense lasers can be challenging. Solid optic equipment can be damaged, and shaping pulses to particular profiles can be expensive. However, plasmas offer many options to shape and manipulate high power lasers, having highly tunable optical properties and no damage threshold. This image shows the results of a 3D particle-in-cell simulation of a spatiotemporally coupled laser pulse compression. The 3D rendered surfaces show snapshots of the laser pulse, coloured according to the amplitude. The lower plane shows the intensity distribution through each snapshot, and the rear plane shows the plasma electron density at the final snapshot. The pulse is compressed uniformly in all directions down to only a single wavelength, accompanied by a huge increase in intensity, over 150 times the initial. Further attempts to compress the pulse cause it to collapse. However, the pulse remnant re-emerges from the collapse site, and even undergoes further collapses.

February



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WINNING IMAGE ENTRY



Turbulence-resolving simulation of the wake behind two in-line wind turbines

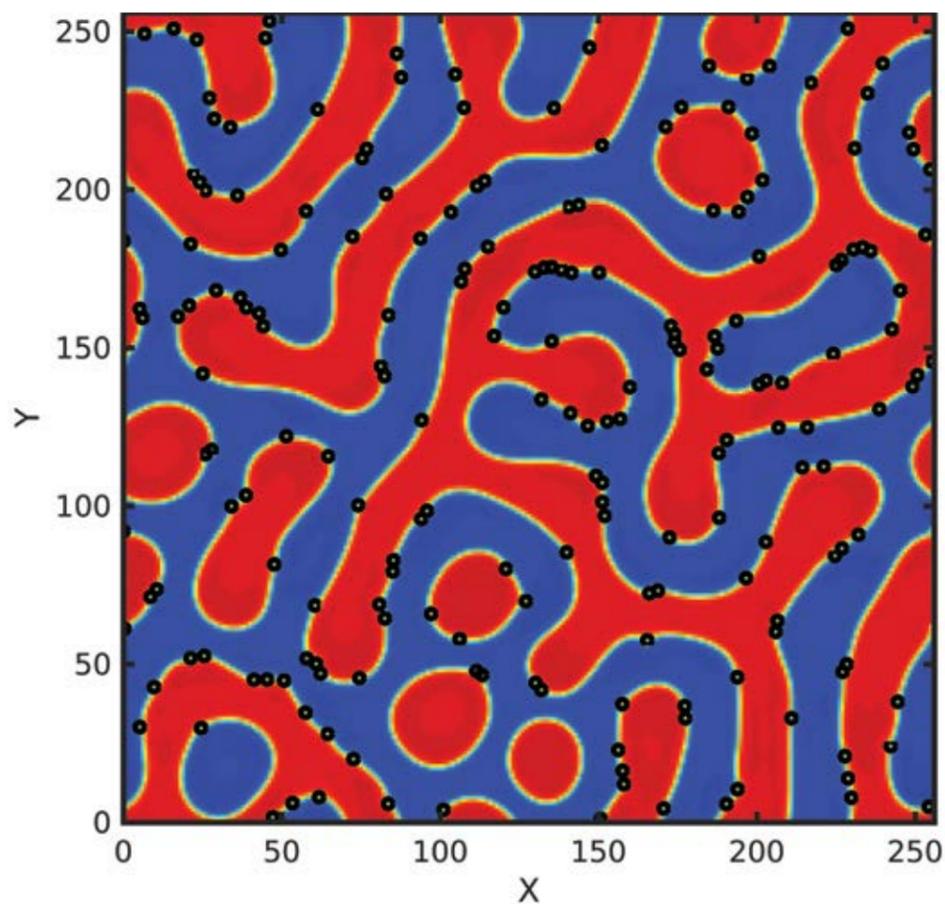
Georgios Deskos, Department of Aeronautics, Imperial College London

Vortical structures generated in the wake of two in-line wind turbines with an incoming velocity of 10 m/s. The simulation was performed on ARCHER using the high-order finite-difference flow framework WInc3D/Incompact3d. The wind turbines are modelled using an actuator line model. Photos are not enhanced.

March



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Circular nanoparticles segregating to the interface between lamellar diblock copolymer domains

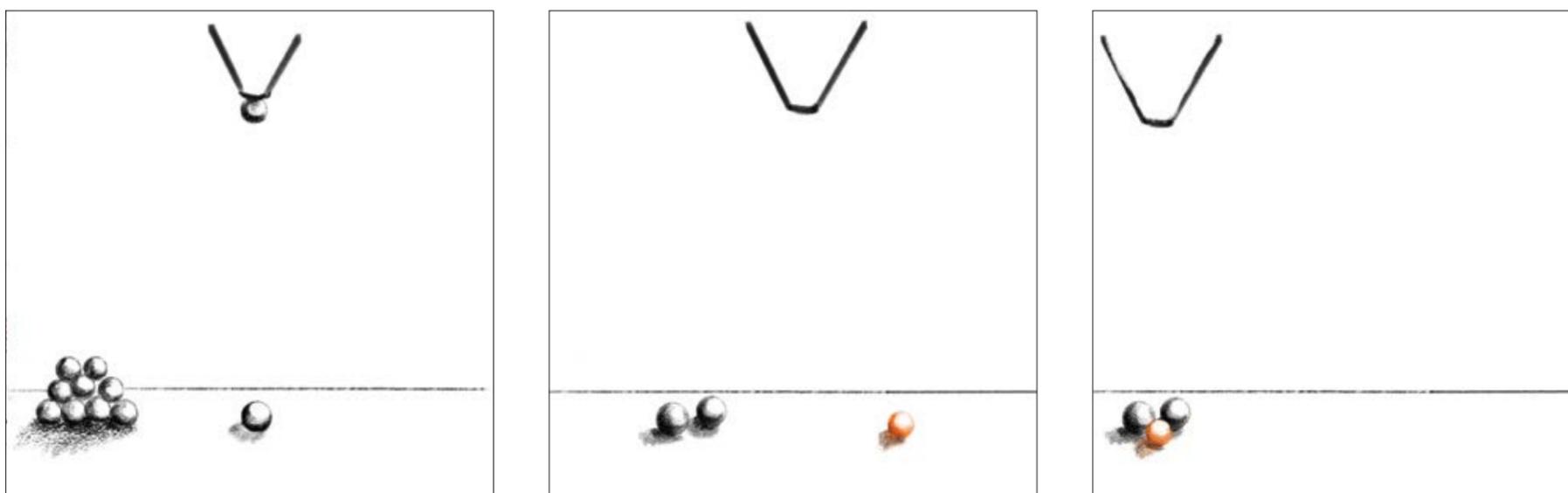
Javier Diaz, University of Lincoln,
School of Mathematics and Physics

Colloidal nanoparticles can be mixed with diblock copolymers to produce highly ordered polymer nanocomposite materials. This still image (taken from a video) shows a simulation of a low concentration of colloids that segregate to the interface between a symmetrical lamella-forming diblock copolymer. The result of this co-assembly is a system with highly localized colloids.

April



MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY	SUNDAY
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Schematic representation of an atom-by-atom building process of nanostructures using purely mechanical forces of an atomic force microscope (AFM) and atomically sharp tips

David Abbasi Perez, King's College London, Department of Physics

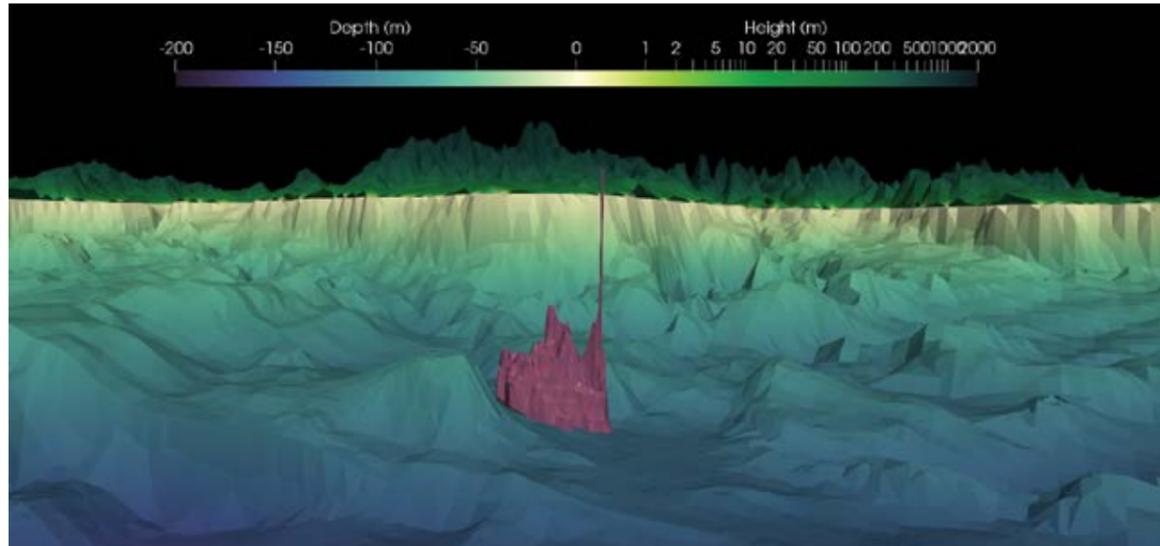
This little cartoon represents a complicated mechanism in which a crane-like device is capable of picking up and depositing one adsorbed atom at a time on the surface and repeating this process many times in order to build 3D nanostructures. This full picking-deposition cycle is key in order to build 3D nanostructures on an atom-by-atom basis using purely mechanical forces of an atomic force microscopy (AFM). This is known as mechanochemistry. The atomic crane is an atomic force microscopy oscillating tip and the material is Gallium Arsenide (GaAs). Although extremely difficult from an experimental point of view, simulations run on ARCHER show that this process is in principle possible. The animation has been created frame-by-frame using the open source code Krita.

May



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WINNING VIDEO ENTRY



Hypersaline sea surface release and propagation under tidal conditions in the northern North Sea

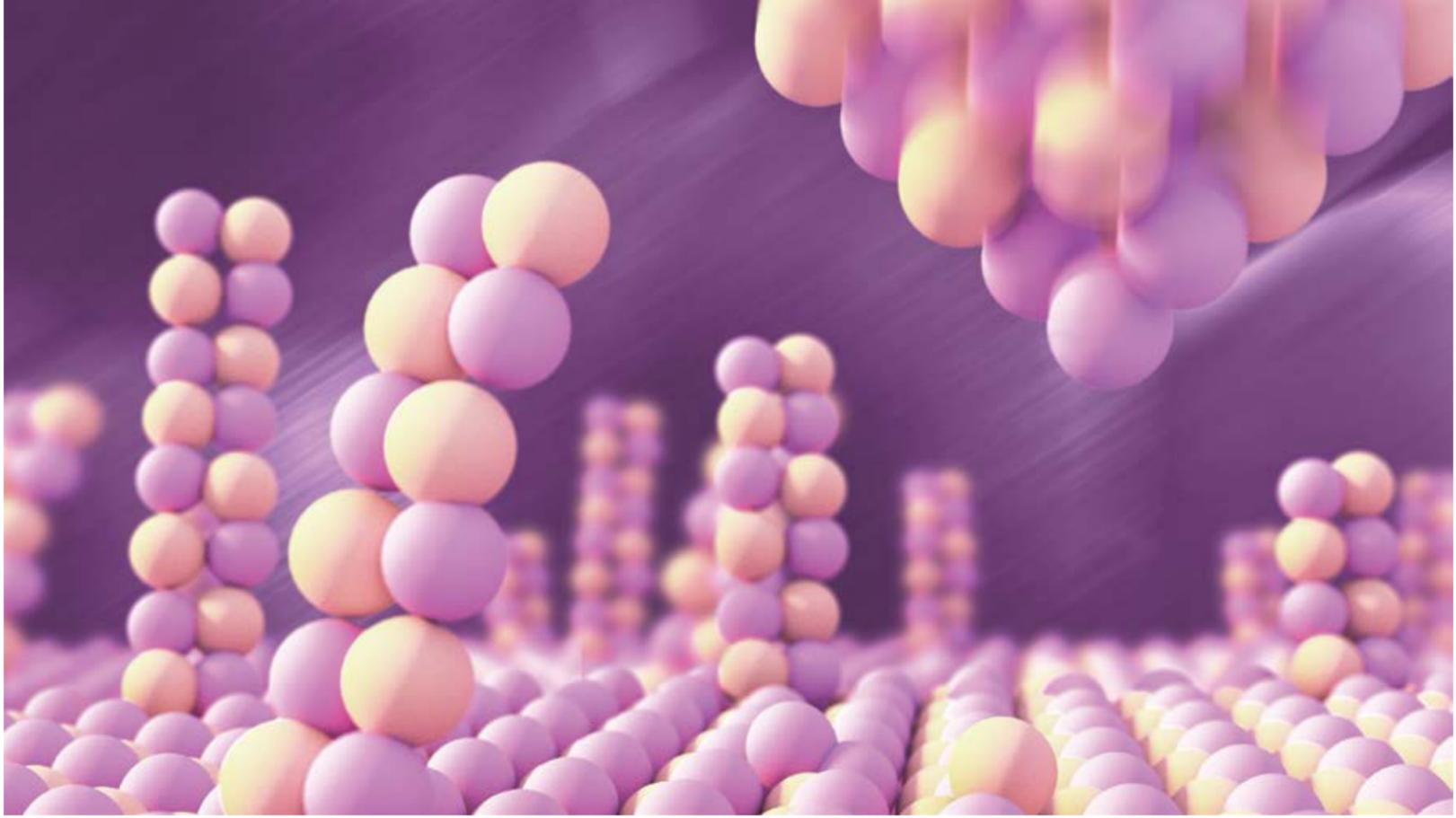
Pierre Cazenave, Plymouth Marine Laboratory,
Marine Ecosystem Modelling and Prediction

A hypersaline point source is set up within an FVCOM model of a region in the northern North Sea. The very salty water is denser than its surroundings and so plummets to the sea bed in a single narrow column. Once at the bottom of the sea, the tides move and mix the salty water making it spread around the seabed, until it is mixed to the point it is indistinguishable from the rest of the water in the North Sea.

June



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Artistic representation of an atom-by-atom building process of 3D nanostructures using purely the mechanical forces of an atomic force microscope (AFM) and atomically sharp tips. The material is Gallium Arsenide (GaAs)
 David Abbasi Perez, King's College London, Department of Physics

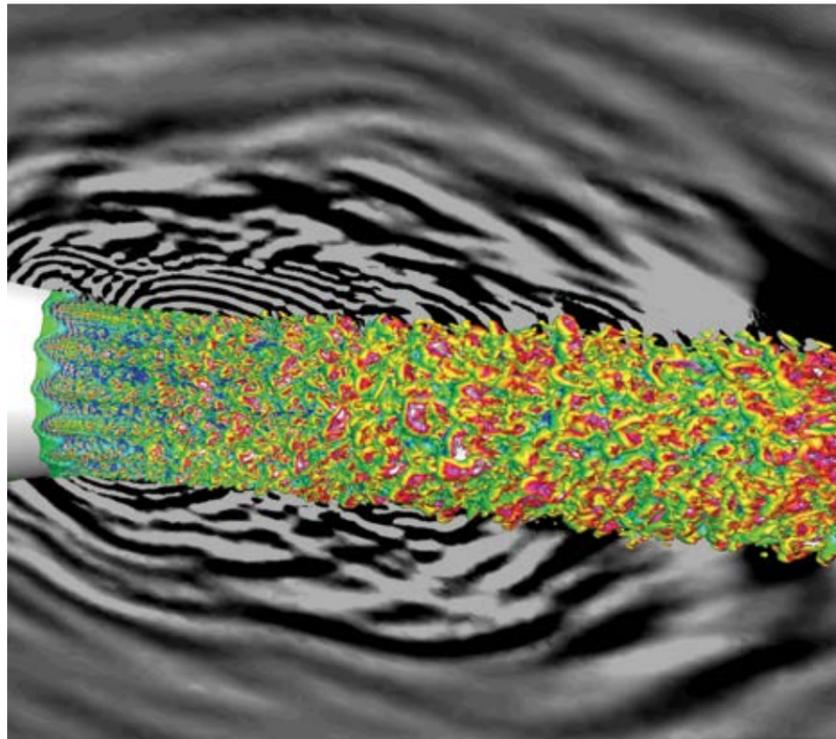
This is an artistic representation that shows an oscillating atomically sharp tip capable of picking and dropping vertically either gallium or arsenic atoms indistinctly in a reversible way in order to build 3D nanorods, using purely mechanical forces. This tip could be seen as an atomic crane and the ultimate objective will be to create 3D nanostructures on a GaAs surface. The tip, at the top right part of the image, is an oscillating atomic force microscopy tip, and the vertical columns are the hypothetical nanorods we would like to build, if possible. Calculations run on ARCHER so far have shown that the reversible picking and deposition process of single atoms using purely mechanical forces is possible. The image has been generated using mainly Blender and The Gimp open software codes.

July



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WINNING EARLY CAREER RESEARCHER AND
OVERALL COMPETITION WINNING ENTRY



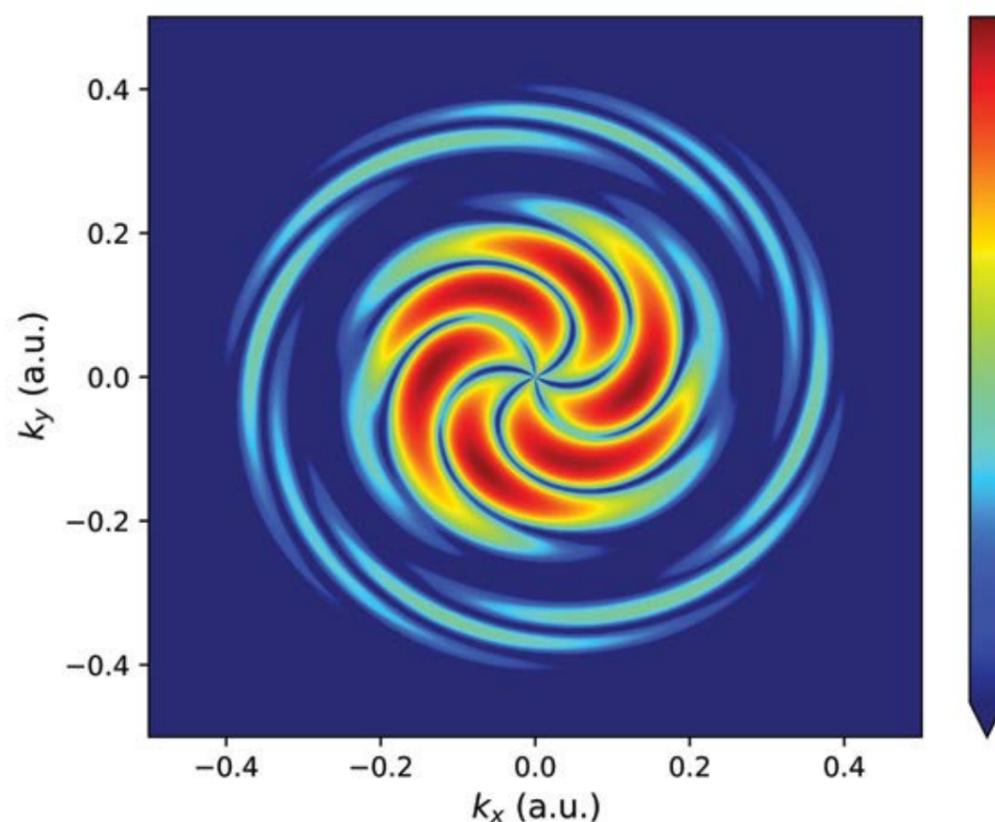
Turbulence-generated noise from a serrated nozzle jet
Zhong-Nan Wang, Department of Engineering,
University of Cambridge

This image shows the broadband noise generated by a turbulent jet from a serrated nozzle. The nozzle serration is used to break up turbulent structures into small scales for noise reduction. The q-criterion shows the turbulent structures and background grey-scale contours shows emitted acoustic waves. Multi-scale phenomena can be seen from the perspectives of both turbulence and acoustics. Acoustic waves are generated at different locations in the near field and interfere as propagating to the far field.

August



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Spiral vortices in photoelectron momentum distributions

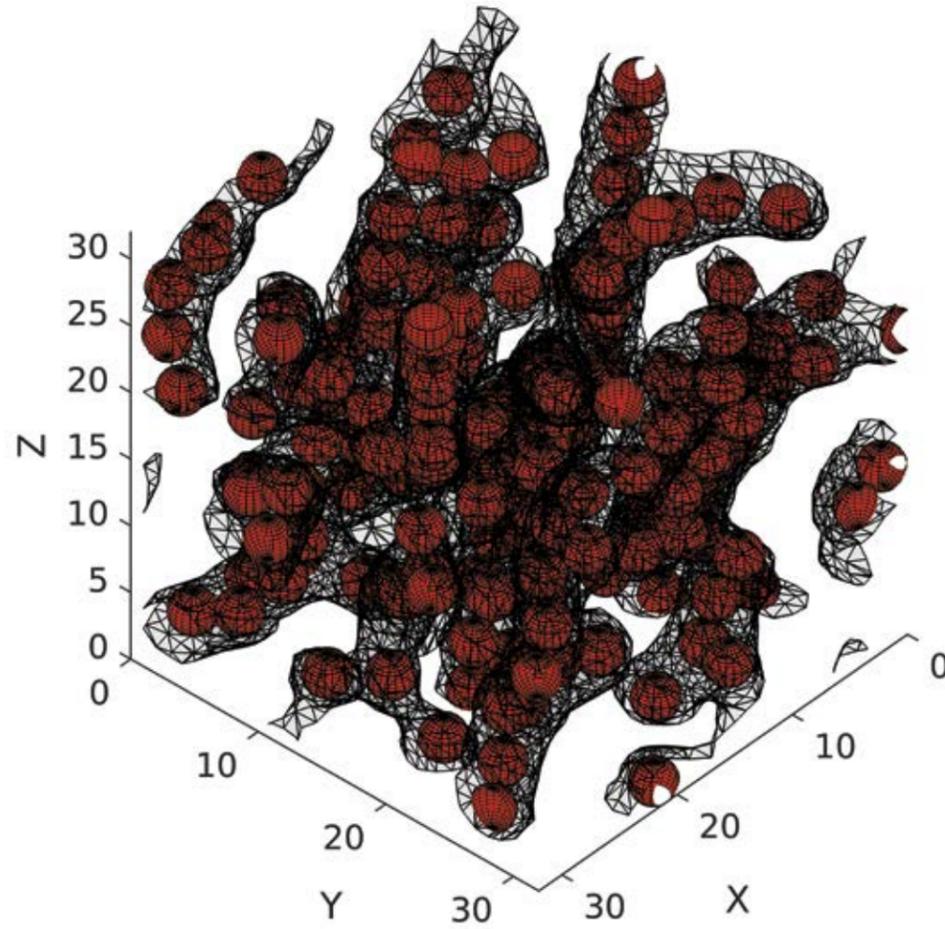
Gregory Armstrong, Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast

The image shows the photoelectron momentum distribution obtained following irradiation of the potassium atom by two counter-rotating circularly-polarized infrared laser pulses. Such pulses induce interference between photoelectron wavepackets which is manifest in the form of spiral vortices in the momentum distribution. Here the inner spiral feature arises from the absorption of three photons from each of the two laser pulses. The opposing helicity of these pulses creates a six-arm spiral interference pattern. The outer spiral feature is the signature of an additional photon absorption from each pulse, resulting in an eight-arm spiral vortex. The calculations were performed on ARCHER using the R-matrix with time-dependence (RMT) codes, which treat interactions between multi-electron atoms and molecules with laser fields of arbitrary polarization.

September



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Spherical nanoparticles in an asymmetrical diblock copolymer

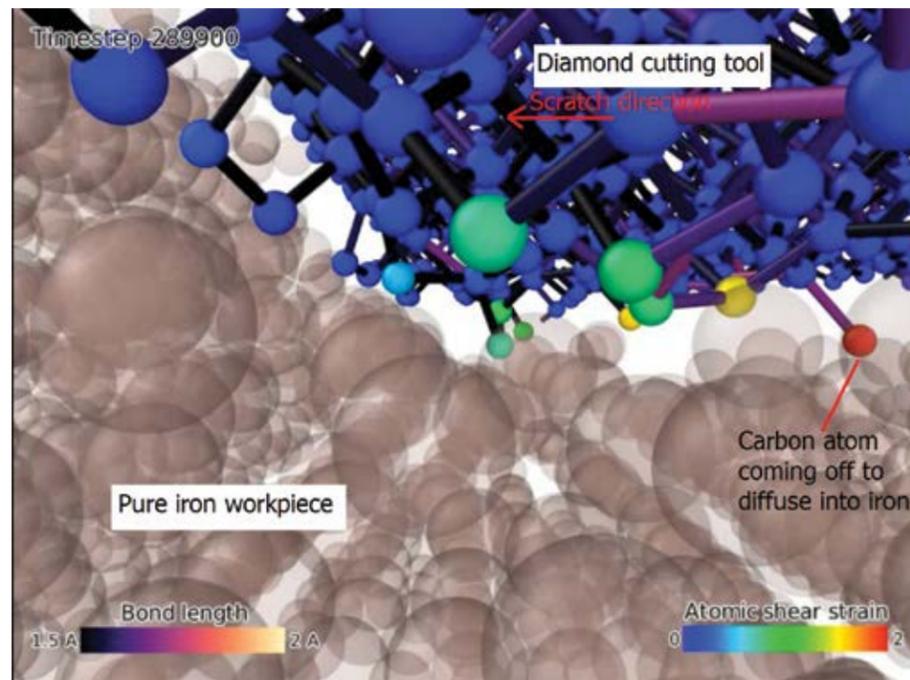
Javier Diaz, University of Lincoln,
School of Mathematics and Physics

Spherical nanoparticles (red) are dispersed in a diblock copolymer mixture. In the absence of particles, a diblock copolymer can phase separate into ordered alternating phases with a periodicity. This makes copolymers a perfect matrix to assembly colloid. Here, the red colloids have an affinity towards the interior of the domains.

October



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Atom-by Atom attrition wear of diamond (carbon atom) while scratching pure iron

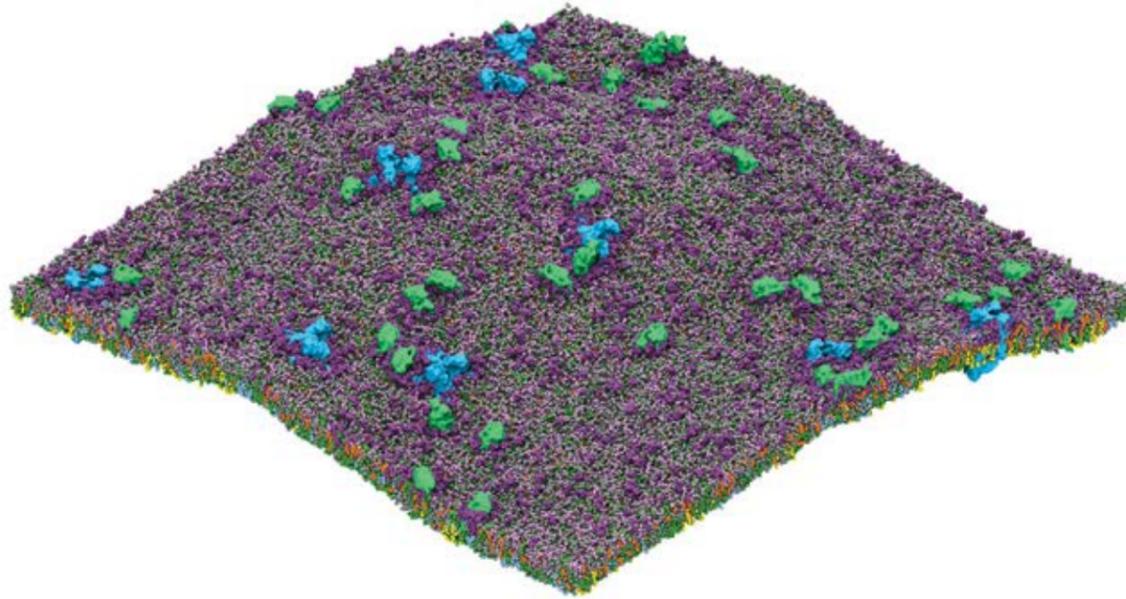
Dr Saurav Goel, Ultra-Precision Engineering, Cranfield University

Despite fifty years of effort, the scientific community has not yet found a convincing explanation for the wear mechanism of diamond during ultra-precision machining of low carbon ferrous alloys or pure iron (a very soft metal). The answer to the wear problem will pave the way to low-cost manufacturing of high-precision moulds, moulds required by handheld gadgets and many other precision applications. This image provides a first direct evidence with high fidelity on the wear of the diamond tool (blue atoms) while scratching pure iron (grey atoms). The time dependent wear of diamond is seen to occur at a timestep of (289900) where one small atom (red colour) experiences unbearable strain and is pulled from diamond. The new findings came from a molecular dynamics simulation on ARCHER using a long range screening bond order potential function fully parametrised for both iron and carbon. This highlights the importance of simulations in practical engineering applications.

November



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Protein clustering on a neuron surface

William Glass, University of Oxford,
Department of Biochemistry

In order for excitable cells to function correctly certain proteins (called ion channels) are critical to allow charged ions to pass across the membrane. The image shows a certain type of ion channel (a voltage-gated sodium channel, blue) that has recently been shown to cluster with other proteins called beta 3 subunits (shown in green). Although it has been shown previously that these proteins interact we have yet to have a clear picture of just what this interaction is and how it can affect the density, location and function of the ion channel. In order to investigate this computationally we used large scale coarse-grained simulations (where 4 'heavy' atoms are represented by 1 'bead'). We constructed a membrane using lipids that are typically found in mammalian cells, with 9 copies of the ion channel and 36 copies of the smaller beta 3 subunit. This system was run for 20 microseconds.

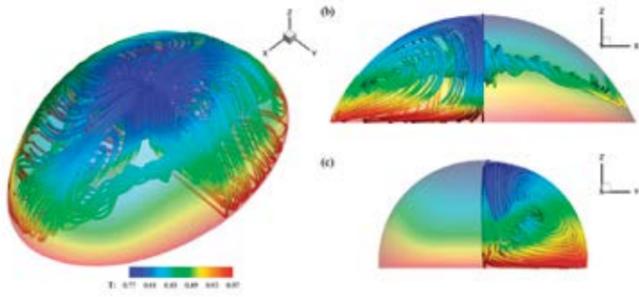
December



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PREVIOUS WINNING IMAGES

2014



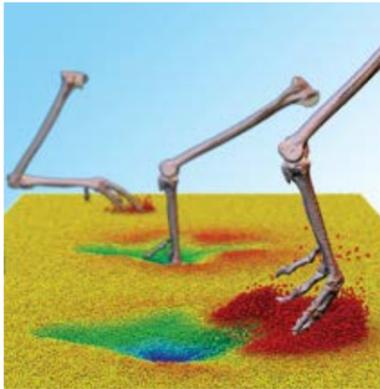
Streamlines illustrating the temperature distribution and emergence of azimuthal currents within the flow of an irregular 3D liquid droplet undergoing phase change
Dr Pedro J. Sáenz, Institute for Materials and Processes, The University of Edinburgh

2015



Music, order and chaos in a combustion chamber
Mr Ivan Langella, University of Cambridge, Department of Engineering

2016



The birth of a footprint
Dr Peter Falkingham, Natural Sciences & Psychology, Liverpool John Moores University

2017



West Scotland Coastal Ocean Modelling System (WeStCOMS) - 3D currents animation
Dmitry Aleynik and Sam Jones, Scottish Association for Marine Science, Physics Department

Notes



All the images in this calendar were submitted by ARCHER users as entries to the ARCHER Image Competition 2018. A gallery of all the images is available on the ARCHER website at <http://bit.ly/2018-Gallery>





THE ARCHER TEAM

www.archer.ac.uk

ARCHER is the UK National Supercomputing Service. The service is provided to the UK research community by the ARCHER Partners: EPSRC, NERC, The University of Edinburgh, UoE HPCx Ltd, EPCC, Daresbury Laboratory and Cray Inc. In addition to running the helpdesk and leading the operations and system activities, EPCC provides the Computational Science and Engineering expertise to support the community in the effective use of ARCHER. For more information visit: <http://www.archer.ac.uk>

