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UNDERSTANDING ICE NUCLEATION AND GROWTH

The formation of ice affects us every day – whether we are preserving food, curing diseases, or predicting the weather. Understanding nucleation and growth, the processes by which water freezes into ice, is critical. However, experiments looking at the formation of ice are incredibly challenging.

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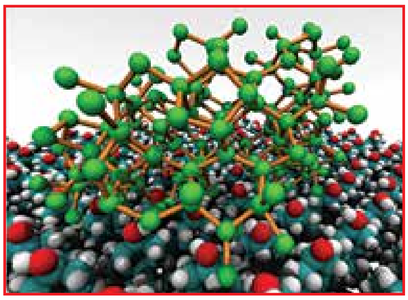
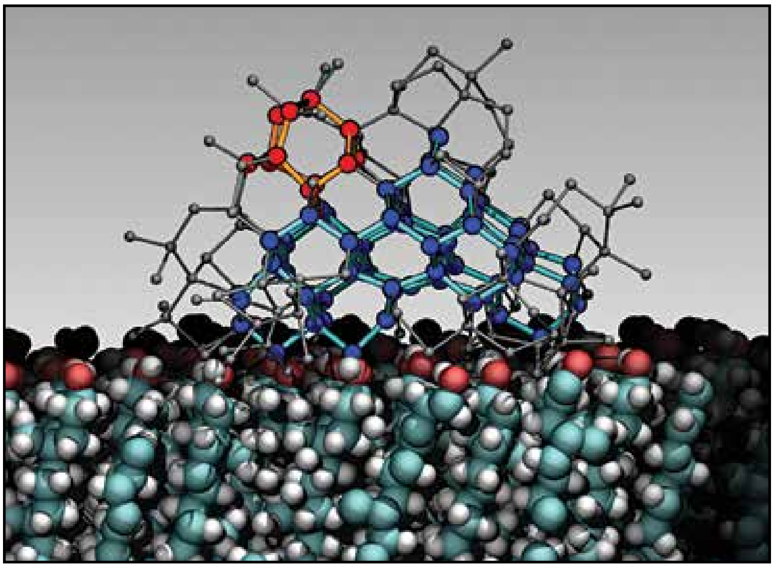


Ice nucleation is a microscopic process that happens on very small length and time scales. It takes only nanoseconds, and newborn ice crystals can be only a few nanometres in size. This means that even state-of-the-art experimental techniques are not able to unravel the molecular-level details of this phenomenon.

Researchers have used ARCHER to simulate how ice forms. These simulations give an unprecedented insight into the formation of ice on a molecular level. This knowledge is key to both the academic community and many aspects of industry.



The benefits of understanding how ice forms are many:

- Atmospheric scientists can take advantage of insights into ice formation. They can see how ice forms on substances such as mineral dust, and predict the impact of this on our atmosphere. This will allow them to improve climate models, with important consequences for the fight against climate change.

- Cryobiologists in the Pharma, Biotech & Healthcare industries can use the outcomes of this research to tailor and improve existing cryopreservation and cryotherapy techniques. This is thanks to the microscopic information about the mechanisms of ice formation on biological matter.

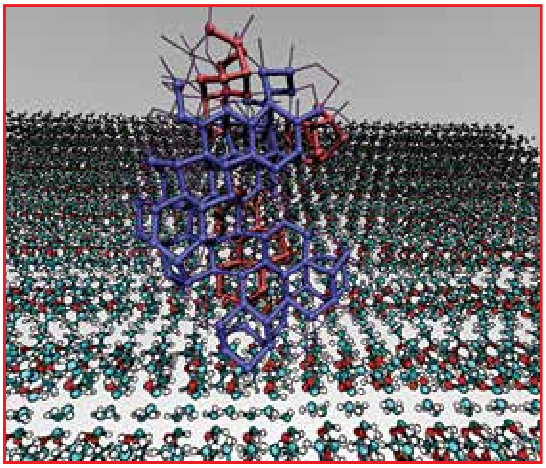
- In the aerospace industry, it is extremely important to understand why and where ice will form. If ice is allowed to form on crucial components, such as joints or flanges, this can have catastrophic consequences. This research will help us to avoid these sorts of accidents.

The UCL/Warwick based research group has been doing atomistic simulations of ice nucleation. These will guide experiments by providing microscopic insight into the formation of ice.

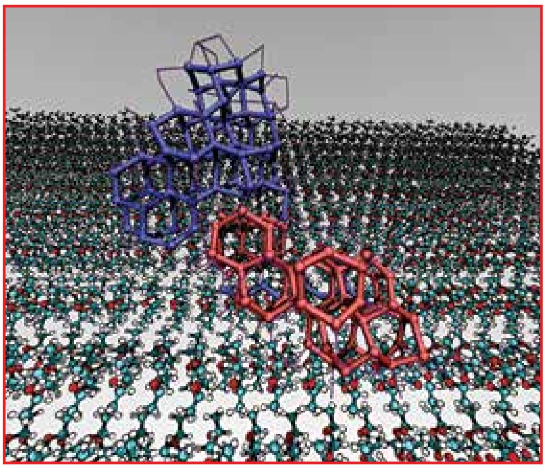
Simulating ice is notoriously challenging, as it is very difficult to convince computer models of water to freeze. In this experiment, researchers used enhanced sampling techniques to allow them to simulate ice formation. However, simulations of ice nucleation are still incredibly computationally expensive. A High Performance Computing facility like ARCHER allowed researchers to take advantage of massively parallel computation.

Most of the water found in nature is contaminated in some way, often by several different chemicals. To truly understand ice formation, we need to understand how impurities affect the nucelation process. Now that ARCHER has helped to provide us with an understanding of the underlying process, this important work can begin.

Parallelisation on the scale of ARCHER meant that the researchers were able to get the water model to freeze and get results in a reasonable time. This makes a facility like ARCHER invaluable. These kind of simulations cannot be done anywhere else within the UK, so ARCHER is just the right tool for the job. The researchers' use of cutting-edge enhanced sampling techniques showcases the power of HPC and ARCHER.



The knowledge we have gained in simulations of ice formation has significant implications on research in many areas. As ice affects many aspects of our society, the knowledge gained here will inform future research in multiple areas. The researchers plan to expand the scope of their experiments to include ice forming on living structures, such as cell membranes.



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About ARCHER

ARCHER is the UK National Supercomputing Service. The service is provided to the UK research community by EPSRC, UoE HPCx Ltd and its subcontractors: EPCC and STFC's Daresbury Laboratory, and by Cray Inc. Laboratory.

The Computational Science and Engineering (CSE) partners provide expertise to support the UK research community in the use of ARCHER, and researchers can also apply for longer-term software development support through the Embedded CSE (eCSE) programme. The ARCHER CSE partners are EPSRC and EPCC at the University of Edinburgh.

The Case Study Series

The ARCHER service facilitates high quality science from a broad range of disciplines across EPSRC's and NERC's remits. The outcome is science that generates significant societal impact, improving health and overall quality of life in the UK and beyond. This science influences policy and impacts on the UK's economy.

This case study is one of a series designed to showcase this science. It has been produced as part of the ARCHER CSE service, supported by EPSRC research grant No EP/N006321/1.

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