archer2

Engineering clean water by freezing: Using vibrations for desalination

multiscale flow X

Institute for Multiscale Thermofluids

cirrus

UKRI Engineering and Physical Sciences Research Council

Swansea University Prifysgol Abertawe

THE UNIVERSITY of EDINBURGH

Ice formation is central to a surprisingly wide range of technologies: from preserving food texture and protecting biological samples, to preventing ice damage in microfluidic devices and producing clean water. Yet despite its scientific and technological relevance, wielding control over *when* and *where* ice forms remains an open scientific challenge. Researchers from the University of Edinburgh and Swansea University have used the computational power of ARCHER2 and Cirrus to gain new insights into this process, and in particular how surface vibrations can be used to control when and where ice forms.
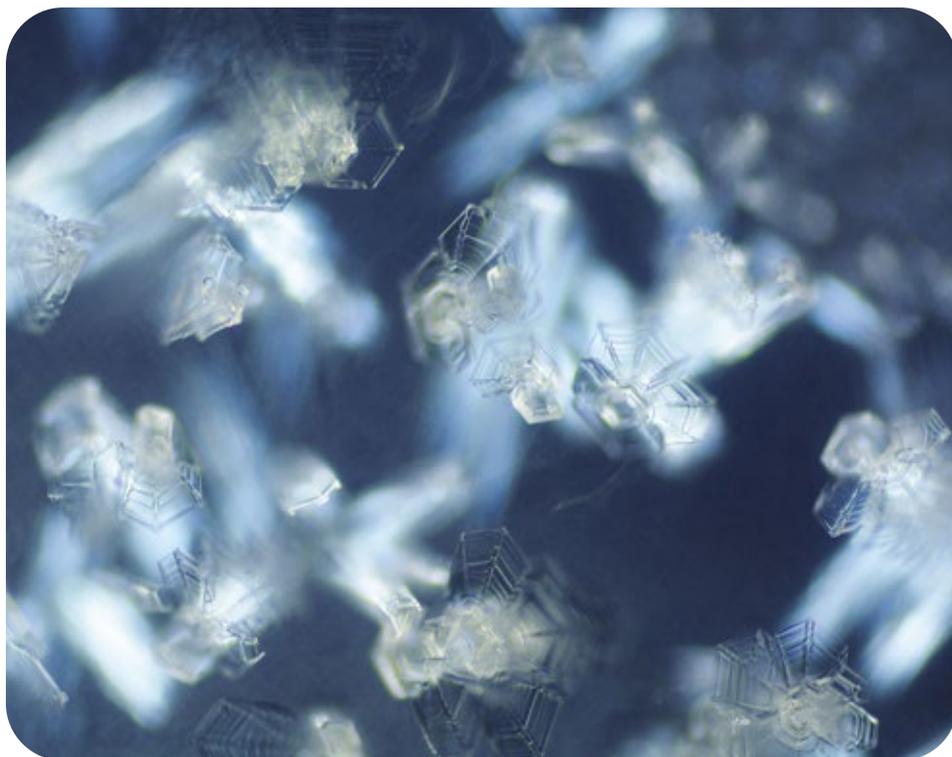
Background and Motivation

The demand for freshwater is rising, but conventional desalination technologies can be energy-intensive. Freeze desalination (FD) offers an alternative route, separating water from brine by partially freezing the solution; the ice crystals can then be removed and melted to yield pure water (Fig. 1). However, for FD to become cost-effective, we need to be able to produce and control ice growth reliably and inexpensively.
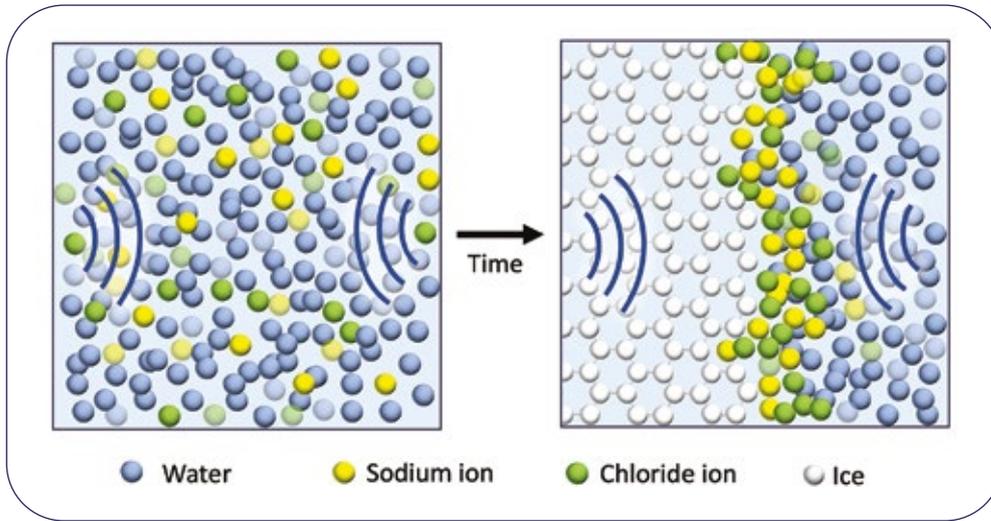

Figure 1: Molecular insights into freeze desalination. As ice crystals (white spheres) grow from salt water, the solid ice structure preferentially incorporates only water molecules (blue spheres), actively rejecting the salt ions (sodium: yellow; chloride: green) into the surrounding liquid brine. This segregation allows the pure ice to be harvested as fresh water.

In conventional freezing, a liquid is cooled until many tiny ice crystals comprising a few water molecules each, referred to as *nuclei*, suddenly appear. Such *nucleation* events produce a slurry of small, irregular crystals that are difficult to separate or control. In contrast, for FD large and well-formed ice crystals are desirable because they can be easily separated from salty brine and washed to provide drinking water. However, achieving this ideal crystal distribution is challenging. Experiments over the past 75 years have shown that high-frequency ultrasound can dramatically change how ice forms, resulting in crystal distributions favourable for FD, but the mechanisms have been the subject of debate. Some studies attribute the effect to cavitation - the violent collapse of bubbles - while others suggest more subtle changes in the liquid structure may be responsible. Because nucleation starts at the nanoscale and unfolds on nanosecond time scales (i.e. billionths of a second), these processes are extremely difficult to observe directly in the lab. This is where High Performance Computing (HPC) resources like ARCHER2 become essential.

Demystifying Vibration-Induced Ice Nucleation

Ice nucleation – the fundamental first step in freezing – is essential to many systems of scientific and technological relevance (Fig.2). In this recent project, the research team turned to molecular dynamics simulations to watch ice nucleation unfold molecule by molecule. They considered a simple but widely relevant configuration: a thin layer of supercooled water confined between two flat surfaces. One surface was kept fixed, while the other was made to vibrate back and forth, mimicking how an acoustic wave would shake the walls of a microscopic channel or pore. Using a coarse-grained molecular model of water, they filled this nanoscale "sandwich" with about sixty thousand water molecules and cooled them down to 50 degrees below freezing, where the liquid is *metastable* relative to the ice, meaning that it would freeze if given the smallest push. The researchers then applied surface vibrations at a range of frequencies and amplitudes, tracking when and where ice nuclei first appeared.
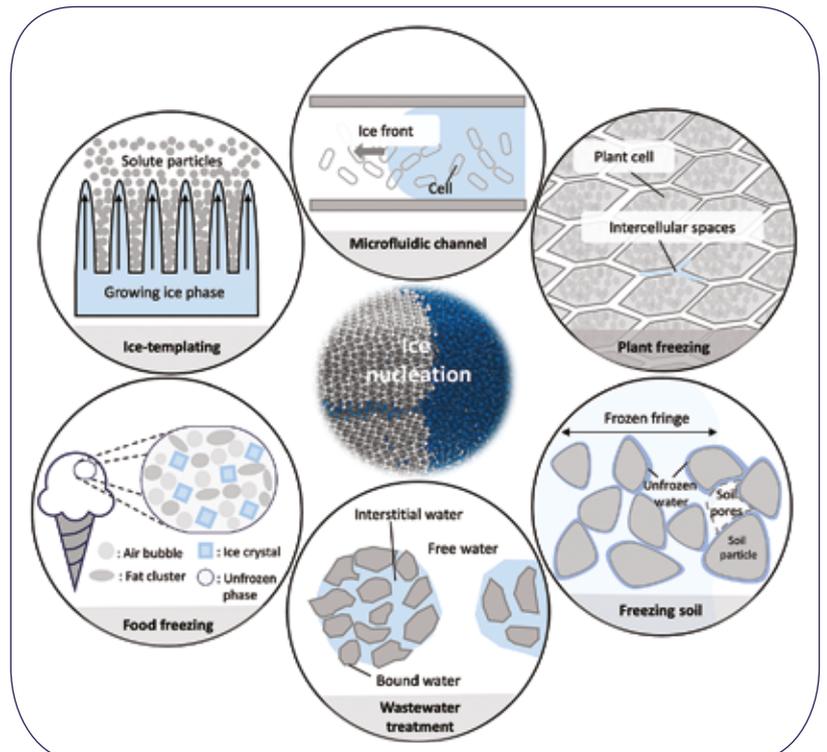
Figure 2: Examples of scenarios involving ice nucleation in confined systems, i.e. pores.

Key Scientific Insights

By running a large number of these complex simulations for a hundred nanoseconds at a time, the research team was able to understand how the outcome of freezing depends on vibration parameters. They observed complete, partial, or no nucleation, as well as the previously observed formation and collapse of cavitating bubbles at larger amplitudes.

Crucially, it was observed that in the nucleation cases, ice always originated at the vibrating or fixed surfaces, rather than in the bulk liquid (i.e. away from the walls). The vibrating wall periodically pulls away from the liquid, subjecting the thin water layer adjacent to the solid to strong tension (or *negative* pressure). During these brief moments, small ice-like clusters are much more likely to form and grow. When the wall moves back and compresses the liquid, many of these clusters melt again, but some are large enough to survive and grow over many vibration cycles (Fig.3).

By analysing the local pressure, it can be shown that it is the magnitude of this negative pressure, rather than the positive pressure associated with compression or bubble collapse as previously suggested, that controls ice nucleation. Increasing the vibration amplitude increases the peak value of the measured negative pressure in a nearly linear fashion, up to the point where cavitation begins. Frequency plays a different role: if the wall vibrates too quickly, the water does not have time to reorganise between cycles, and the transient ice-like structures cannot develop into stable nuclei. This leads to a clear frequency cut-off above which nucleation becomes unlikely even if the amplitude is large. To investigate whether these observations fitted a general trend, a simple strain measure was introduced: the vibration amplitude divided by the thickness of the water layer. When all of the data was replotted in terms of this strain, the research team found that results from different system sizes mapped onto the same master curve. A critical strain of about 4% was sufficient to trigger nucleation; beyond about 9%, cavitation dominated and suppressed ice formation. This apparently universal and *scale-free* description is particularly valuable because it can be applied not only to the nanometre-scale systems which can be simulated directly, but also to micron-scale channels and industrial devices.
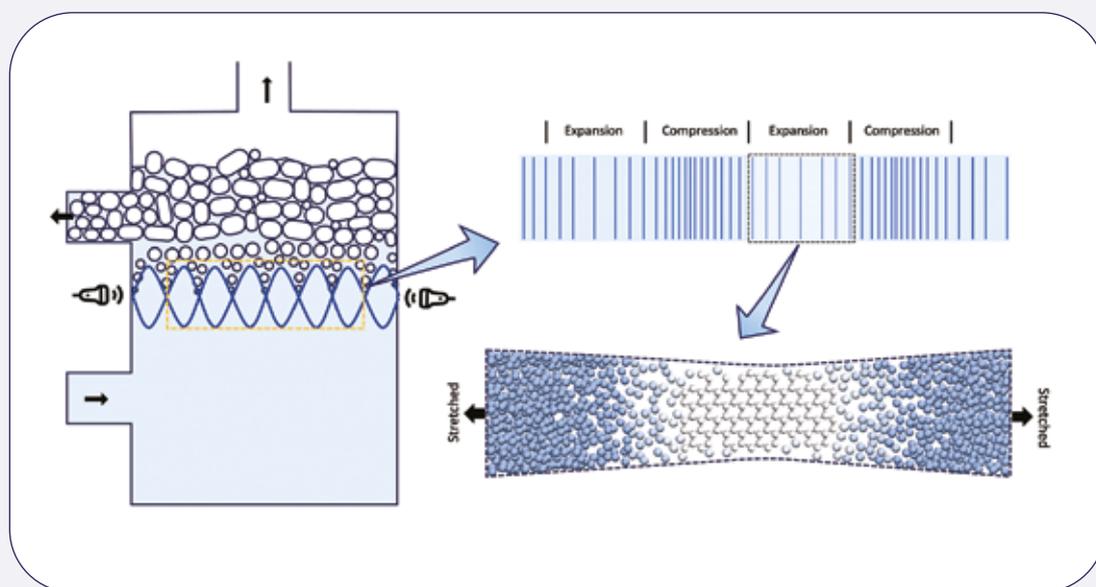
Figure 3: A diagram illustrating the mechanism of vibration-induced ice nucleation. Ultrasound waves passing through the supercooled water create alternating regions of compression and expansion. The areas of expansion effectively "stretch" the water, generating a negative pressure zone that triggers the ice formation.

From Fundamental Physics to Freeze-Desalination

The picture that emerges from this work is straightforward but powerful: a vibrating surface can be used as a nanoscale "piston" to periodically pull on a liquid, generating brief bursts of negative pressure that encourage ice nuclei to form on demand. Because the key control parameter is strain rather than absolute size, the same physics should hold in much larger systems. The research team's current work builds directly on this insight and targets FD, in which ultrasound drives the formation of a slurry of pure ice crystals from seawater. To keep costs low, FD needs relatively few, large ice crystals that are easy to separate and wash. Conventional operation tends to produce many fine crystals instead, making separation difficult and reducing overall efficiency. Preliminary experiments suggest that ultrasound can change the crystal size distribution, but there is little guidance on how to choose frequency, intensity or salinity. The simulations on ARCHER2 provide exactly the kind of molecular-level understanding needed to turn this idea into an engineering tool.

In this project the research team extended their vibration-controlled freezing framework to saltwater (Fig. 1). They examined how dissolved ions modify the structure of supercooled water near vibrating surfaces, how salinity shifts the strain thresholds for nucleation and cavitation, and how salt gets incorporated or rejected during crystal growth. The team is currently addressing four interlinked questions: how ultrasound changes nucleation rates in salty water; how this effect depends on salt concentration; how it can be used to steer crystal growth toward larger, more uniform ice particles; and how these mechanisms can be translated into design rules for practical FD units.

Figure 4: Ice formation in vibrating nanopores: Molecular dynamics simulations show that surface vibrations generate negative pressure in confined supercooled water, promoting ice nucleation.

National Importance and Future Directions

This research sits at the intersection of water engineering and desalination (application area), acoustics (controlling/design parameter), and nanoscale thermodynamics (underlying mechanisms). It directly supports national priorities in water security, low-carbon technologies and engineering across length-scales. By combining fundamental molecular simulations with application-driven goals, the work contributes to EPSRC's vision of designing from atoms to applications.

References:

P. Chen, R. Pillai, and S. Datta, "Nanoscale insights into vibration-induced heterogeneous ice nucleation," Nanoscale 17, 14172–14182 (2025).

Authors:

Pengxu Chen (The University of Edinburgh)
Santiago Romero-Vargas Castrillon (The University of Edinburgh)
Rohit Pillai (The University of Edinburgh)
Saikat Datta (Swansea University)

Contact Details:

Pengxu Chen **Pengxu.chen@ed.ac.uk**
Santiago Romero-Vargas Castrillon **Santiago@ed.ac.uk**
Rohit Pillai **R.Pillai@ed.ac.uk**
Saikat Datta **saikat.datta@swansea.ac.uk**

About ARCHER2

ARCHER2 is the UK's National Supercomputing Service, a world class advanced computing resource for UK researchers. ARCHER2 is provided by UKRI, EPCC, HPE and the University of Edinburgh. ARCHER2 is the latest in a series of National Supercomputing Services provided to UK researchers.

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