Novel algorithm simulates water evaporation at the nanoscale

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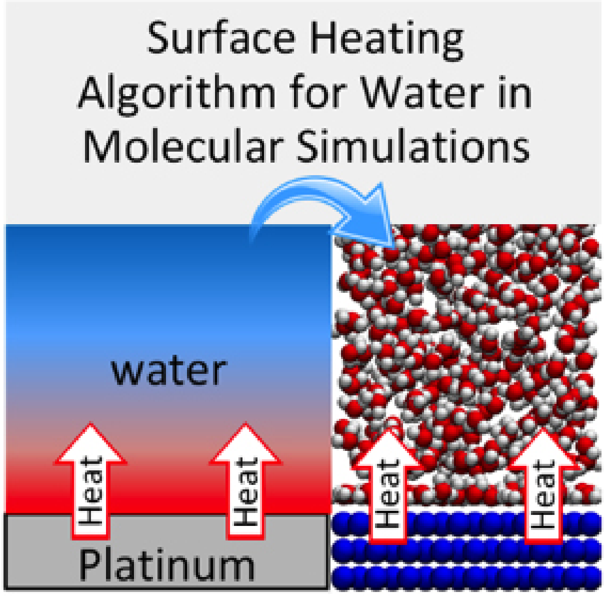

We are all familiar with boiling a pot of water—flame from a stove heats the base of a metal pot, the metal transfers the heat to the water, and the temperature goes up and up until the water boils. Professor Shalabh Maroo and graduate student Sumith YD are looking closer—much closer. They are looking at heat transfer in water at the nanoscale, where the heat from the pot's atoms transfers to the atoms that make up water.

The evaporation of water that occurs when it meets a hot surface is understood in continuum theory and in experimentation. Before now, researchers were unable to study it at nanoscales in molecular simulation. YD and Maroo's algorithm has made that possible, and their paper, "Surface-Heating Algorithm for Water at Nanoscale," has garnished notable attention in the *Journal of Physical Chemistry Letters*.

Within their paper, the pair details their development of a new algorithm that simulates the evaporation of water at the molecular scale that matches theoretical, numerical, and real-world observations. In doing so, the team has provided a molecular dynamics tool that allows for the study of various heat transfer problems at the nanoscale, including understanding and utilizing passive liquid flows.

"By capturing realistic differential thermal gradients in water heated at the surface, our algorithm can be an incredibly valuable tool for studying a range of heating and cooling problems. It's also simple enough to be easily integrated into various molecular simulation software and user codes," describes Maroo.

This research is part of Maroo's CAREER award research, in which he is investigating the fundamental physics associated with nanoscale meniscus evaporation and passive liquid flow to remove large amounts of heat from small surfaces in very short amounts of time. This work aims to provide rapid and efficient cooling of next-generation computer chips and energy conversion devices.

Provided by Syracuse University

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