

By tracking water molecules, physicists hope to unlock secrets of life

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(PhysOrg.com) -- Compared to any other liquid on Earth, water behaves in strange and unexpected ways, yet its unusual properties enable and protect life as we know it. By tracking individual water molecules in a "supercooled" state, scientists find what explains one of water's most notable and life-saving features: its astounding capacity to resist gaining or losing heat.

The key to life as we know it is water, a tiny molecule with some highly unusual properties, such as the ability to retain large amounts of heat and to lose, instead of gain, density as it solidifies. It behaves so differently from other liquids, in fact, that by some measures it shouldn't even exist. Now scientists have made a batch of new discoveries about the ubiquitous [liquid](#), suggesting that an individual water molecule's interactions with its neighbors could someday be manipulated to solve some of the world's thorniest problems — from agriculture to cancer.

The work, led by Pradeep Kumar, a fellow at Rockefeller University's Center for Studies in Physics and Biology who looks at the role of water in biology, makes it possible to measure how interaction between [water molecules](#) affect any number of properties in a system. It also paves the way for understanding how water can be manipulated to facilitate or prevent substances from dissolving in it, an advance that could impact every corner of society, from reforming agricultural practices to improving [chemotherapy](#) drugs whose side effects arise from their solubility or insolubility in water.

Kumar and his colleagues first tracked individual water molecules in a "supercooled" state (water that remains in liquid form even at below freezing temperatures), during which water's many anomalies are enhanced. "When you put water in a freezer, it doesn't freeze instantaneously," says Kumar. "It takes some time. If you have extremely pure water, then you can go down to about 230

[Kelvin](#) and still have enough time to measure different physical properties of water including the specific heat in its liquid state." Kumar and his colleagues then used theoretical and computational approaches to simulate the activity of these water molecules and measure their interactions with neighbors.

In the liquid state, every water molecule fleetingly interacts with its four nearest neighbors, forming a tetrahedron, explains Kumar. These tetrahedrons, however, are slightly imperfect and the degree to which they are changes as temperature and pressure change, ultimately affecting which individual water molecules partner up with each other. Kumar found that it is the fluctuations in the degree of tetrahedrality that contribute most to one of water's most notable and valuable features — its capacity to resist heating or cooling and thereby regulating and maintaining the temperature of biological systems.

The ability to measure water's shifting degrees of tetrahedrality also gives scientists a means of measuring how much order or disorder each water molecule imparts. The better the tetrahedron, the more order it imparts in the system. "What we have done essentially is define the structural entropy of every molecule in our system," says Kumar. "And since water molecules are constantly moving in space and time, this gives you a way to study the transport of entropy associated with local tetrahedrality — something that has never been done before."

Understanding how individual water molecules maneuver in a system to form fleeting tetrahedral structures and how changing physical conditions such as temperatures and pressures affect the amount of disorder each imparts on that system may help scientists understand why certain substances, like drugs used in chemotherapy, are soluble in water and why some are not.

It could also help understand how this changing network of bonds and ordering of local tetrahedrality between water molecules changes the nature of protein folding and degradation.

“Understanding hydrophobicity, and how different conditions change it, is probably one of the most fundamental components in understanding how proteins fold in water and how different biomolecules remain stable in it,” says Kumar.

“And if we understand this, we will not only have a new way of thinking about physics and biology but also a new way to approach health and disease.”

More information: *Proceedings of the National Academy of Sciences* [online: December 14, 2009](#).

A tetrahedral entropy for water. Pradeep Kumar, Sergey V. Buldyrev and H. Eugene Stanley

Provided by Rockefeller University

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