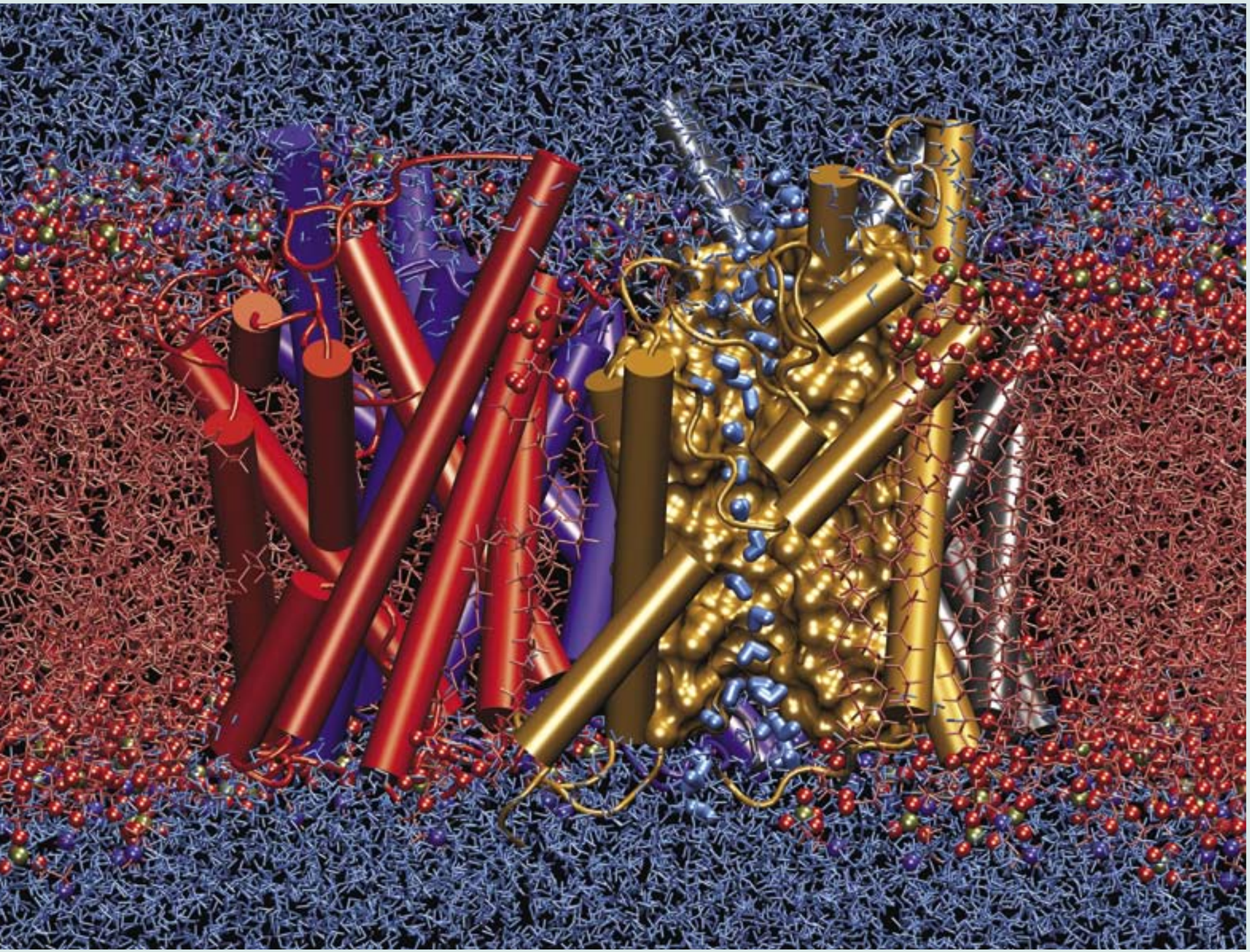

Aquaporin water channel is captured at work in a snapshot taken from a full-atomic molecular dynamics simulation. The depicted system is one of the largest and longest membrane protein simulations ever done, comprising more than 106,000 particles (atoms). The image shows a cell membrane in cross section, separating extracellular water *(top)* from the water inside the cell *(bottom)*. Time on NSF's Pittsburgh Supercomputer Center was used for the computationally intense simulations. (Data from Tajkhorshid *et al.* 2002, *Science* 296:525–530.)

Felice Frankel is a science photographer and research scientist at the Massachusetts Institute of Technology. She is now at work organizing Image and Meaning 2, an MIT conference to be held in Los Angeles in June 2005 (http://web.mit.edu/i-m). Address: c/o American Scientist, *P. O. Box 13975, Research Triangle Park, NC 27709-3975. Internet: felicef@mit.edu*

Sightings

Felice Frankel

When judging this year's Science and Engineering Visualization Challenge contest sponsored by the National Science Foundation, I knew I wanted to share this first-place illustration with American Scientist *readers. Emad Tajkhorshid is a computational biophysicist at the National Institutes of Health Resource for Macromolecular Modeling and Bioinformatics at the Beckman Institute, University of Illinois at Urbana-Champaign. Klaus Schulten directs the Theoretical and Computational Biophysics Group, whose purpose is to develop software for biomedical and other investigators. The most popular software developed, called VMD, was used to generate this image. For more information, go to http://www.ks.uiuc.edu/Research/vmd.*

F. F. Can you explain to readers unfamiliar with molecular biological representations how to read the image?

E. T. The image can be broken into proteins, lipids and water. Small molecules can be shown in an all-atom representation, explicitly showing all atoms and bonds. Biomolecular macromolecules are much more crowded. Showing all atoms and bonds makes the visualization useless. So people have come up with simpler representations. For example, in proteins we can look at the backbone atoms in the polypeptide chain and ignore the side chains of individual amino acids. If backbone atoms are arranged in a helical shape, we show the protein in that region using rods; if we have multiple strands lying next to each other, we show them as ribbons.

Now, in our simulation system, we have a box packed with 106,000 atoms. Naturally showing all of these components in full atomic detail does not get us anywhere, since there are way too many atoms. At the same time, we really wanted to show as much detail as possible. So we used different representations for different parts. Water molecules are shown always using a stick representation (representing the only two chemical bonds in their structure) in light blue. In the membrane region, sandwiched between the two water layers, we see two major components: in the middle an array of four identical proteins (a tetramer) and on the left and right lipid molecules forming the so-called lipid bilayer structure embedding our protein.

F. F. You exaggerate the size of the water molecules as they pass through the channel. Did you think that might be misleading?

E. T. It was indeed one concern we had. The first reaction of some viewers was to ask why we have "different" water molecules inside the channel. It seemed to them that something happens to water as it enters the channel that makes it special. This is both right and wrong, depending on how you look at it. The chemical nature of water molecules does not change. But the configuration of water has indeed been influenced by the channel. In the bulk we have always several water molecules surrounding every single water molecule. Inside the channel, however, water molecules are forced to form a single file. This is not something a water molecule likes, as it loses some of its favorable interactions with other water molecules. This fact turned out to be very important for the selective function of this channel. So we used an exaggerated representation.

F. F. Can you give us some sort of hierarchy of the information you hoped a reader would glean from looking at the image for the first time? It's obvious how "packed" all the molecules are. What else was important to convey?

E. T. The density and complexity of the molecular system was certainly one of our main objectives. The second most important message is the water configuration. The membrane fatty core (shown in red sticks) is very efficiently isolating the water on the two sides. But there is a conduit inside the protein that allows water to get to the other side. The viewer, we hope, sees how closely water interacts with the channel. Also when one pays a little attention, the flip of water molecules at the center of the channel becomes obvious. Water comes in head first, turns 180 degrees and goes out head-last. The oxygen atom at the center of each water molecule is always facing the center of the channel. It's like a ballet in which the dancers who come onto a stage have been asked to face a singer standing in the center of the scene.

Resource: Making Science and Engineering Pictures: A Practical Guide to Presenting Your Work

Felice Frankel