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seeing science

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BY KATHARINE MILLER

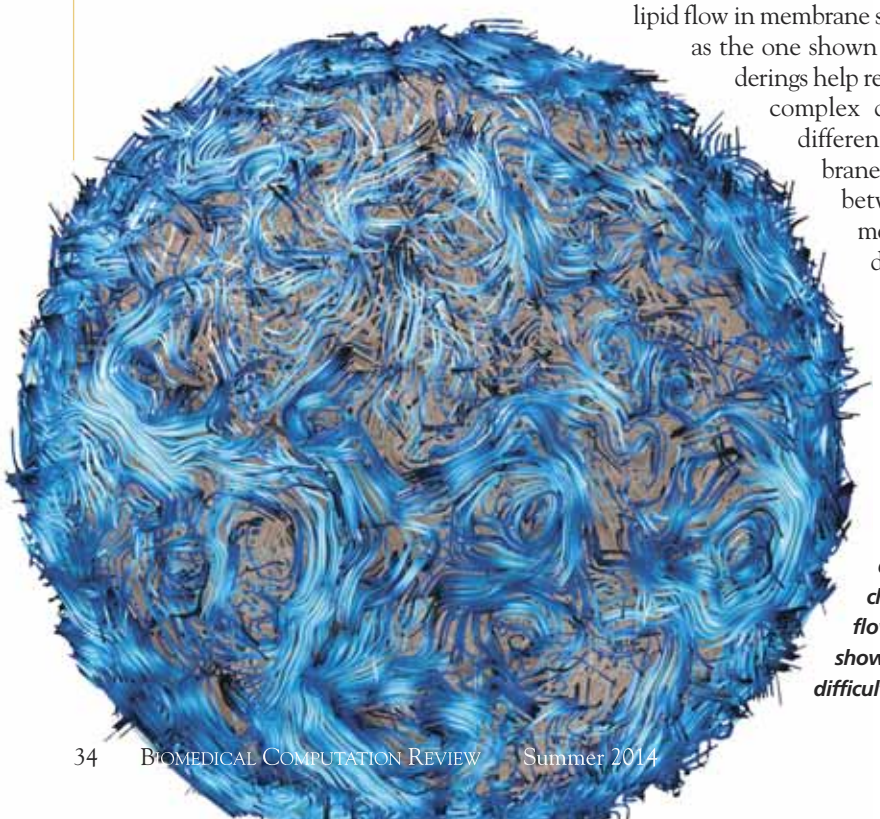
Streamlining Lipids

As computational power grows, researchers can model and simulate larger and larger molecular complexes. To visualize such systems in action, **Matthieu Chavent, PhD**, a postdoc in Mark Sansom's laboratory at the University of Oxford has turned to a physics-based strategy often used to depict atmospheric flows and oceanographic currents. It's called streamline visualization.

"It is really well-adapted to large molecular systems," says Chavent. Indeed, he has used the method to render images of lipid flow in membrane simulations, such as the one shown here. Such renderings help researchers see the complex dynamic among different types of membrane lipids as well as between lipids and membrane-embedded proteins. The insights gained could lead to a greater understanding of how drugs and viruses interact with membranes.

To create the streamlined visualizations, Chavent divides a detailed membrane model into a grid of cells. He then associates a vector to each cell, creating a vector field. The streamline approach connects the vectors together. "Instead of focusing on every lipid, which is quite complicated and may blur the view, we obtain a larger view to focus on the membrane as an ensemble," Chavent says. The approach may also prove valuable for visualizing smaller systems consisting of many molecules, such as water flow around macromolecules, Chavent says.

Chavent is currently developing a streamline visualization plugin that will work with VMD, a popular molecular visualization program. The method is freely available at the following address: http://sbcb.bioch.ox.ac.uk/flows/. □



This streamline visualization, which recently won first place in the Biophysical Society Art of Science Image Contest 2014, displays lipid movement in a spherical vesicle membrane bilayer. The outer leaflet is depicted by colored streamlines—white lines are higher velocity than blue. Brown lines represent the inner leaflet with speed not shown. The rendering is based on a lipid vesicle model developed by Syma Khalid, PhD, senior lecturer in computational chemistry at the University of Southampton. The visualization reveals flowing movements as well as vortices around the proteins (not shown) that move like rafts in a lipid sea. These circular movements were difficult to see using other methods. Courtesy of Matthieu Chavent.