Researchers develop computer model to study cell membrane dynamics

April 8 2008

A cell constantly remodels its fluid membranes to carry out critical tasks, such as recognizing other cells, getting nutrients or sorting proteins. Because membranes are fluid and intrinsically disordered, investigating these and other life-sustaining processes in detail has always been difficult. But a computer model developed by Markus Deserno, associate professor of physics at Carnegie Mellon University, provides a new approach by allowing him to simulate and observe membrane dynamics at a relatively large scale -- hundreds of nanometers. It is at this scale that many critical membrane-mediated processes take place.

Deserno will describe the application of this model to the biophysical problem of vesicle creation on Tuesday, April 8 at the 235th national meeting of the American Chemical Society in New Orleans.

“Our model is coarse-grained,” Deserno said. “You can think of it as an impressionist painting. At a distance, everything looks good. You can see water lilies or ballerinas. But up close, all the details are gone; you just see blotches of color. We’re interested in what’s happening with the water lilies, not the blotches of color,” he added.

With this coarse-grained model, Deserno can accurately capture important large-scale characteristics, like how the membrane bends and curves, which allows him to ask questions that are beyond the atomic resolution but less than the size of an entire cell. His model is also versatile as he can add proteins of interest to the lipid membrane and observe how they interact.

Using this computer model, Deserno and colleagues at the Max Plank Institute for Polymer Research in Mainz, Germany, recently revealed a purely physical mechanism that enables vesiculation — the process by which cell membranes curve around proteins or other cellular cargo to form "vesicles." Without this generic ability to curve its protein-studded membranes and bud off cargo shuttles, a cell couldn't survive.

"Ultimately, understanding the dynamics of vesiculation is key to advancing the design of anti-viral therapies or understanding how protein processing goes awry within a cell and leads to disease," Deserno said.

Deserno and his team created a computer simulation of a cell membrane with a lipid bilayer — a soap-like film made of 50,000 individual lipids molecules — and studded it with 36 evenly spaced and contact lens-shaped disks representing remodeling proteins, which are involved in vesiculation. Then he set the simulation to allow the fluid membrane to fluctuate as it normally would. During the simulation, the artificial membrane began curving in places. In creating curved membrane structures, each disk bent the membrane slightly. This local curvature spread around a disk like a little "halo." When two disks approached one another, the overlapping halos led to an indirect interaction. Thus, while there was no explicit interaction between the disks, these objects indirectly attracted each other via the membrane, Deserno's group found.

"With this work, we provide solid support for a mechanism that has been gaining in popularity recently," Deserno said. "To date, no one has demonstrated at the biophysical level exactly what most people have come to accept as evident — that remodeling proteins can indeed aggregate and facilitate vesiculation based on their curvature imprint alone. Our simulations show that proteins need not interact directly to drive this critical process."

Understanding how vesiculation physically operates should make it

easier in the long run to rationally design and deliver drugs to individual cells, according to Deserno. “This is the biggest practical value of our research. Now that we have a proposed mechanism, we can subject it to well-posed questions, such as why certain proteins are always present during vesiculation.”

In addition to investigating the process of membrane mediated interactions in computer simulations, Deserno, together with colleagues Jemal Guven at the Universidad Nacional Autónoma de México and Martin Müller at the École Normale Supérieure in Paris, has developed powerful theoretical tools to study the transport of stresses and forces through curved membranes.

Source: Carnegie Mellon University

Citation: Researchers develop computer model to study cell membrane dynamics (2008, April 8) retrieved 25 April 2024 from https://phys.org/news/2008-04-cell-membrane-dynamics.html

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