Atomic-scale model unravels ion channel gating

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U. ILLINOIS (US)—Nerve cells power human intelligence and behavior through electrical signals that rely on potassium and sodium ion channels to do their job, and an important part of that biological process involves a gating mechanism for generating and controlling the signals in those channels.

Understanding how that gating process actually works has confounded scientists for decades. Now researchers have visualized and explained how this mysterious process works at the molecular scale.

Scientists at the University of Illinois's Beckman Institute used molecular dynamics simulation software they developed called NAMD to create an atomic scale model of the structures and processes involved in this critical biological function.

They describe their work and findings in *Biophysical Journal*.

The researchers write that the mystery revolved around the fact that the "channel involves a protein with few charged amino acids that seem to be only weakly coupled energetically to an electrical potential gradient across the cell membrane."

Their computer modeling using NAMD—powered by a powerful array of computers that permit the large scale dynamic simulations required to create atomistic models—led to the description of what is called a voltage gating charge that enables the process of nerve cell signaling in voltage-activated channels.

Their simulations revealed that "the potential gradient is focused by the channel protein to a very narrow region such that its value is much larger than anticipated.

The protein was also seen to arrange its charged amino acids sensing the gradient in an unusual helix, a so-called 3-10 helix, that aligns charges perfectly while at the same time inducing a motion that opens and closes the channel."

The researchers' computational findings about the gating current were validated by empirical observations.

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