Anton shows how water leaving, re-entering potassium channel structure delays return to active state

The potassium channel activates nerve and other electrically active cells by allowing electrically charged potassium ions across the cell membrane. In its normal function, it then has to turn that flow of ions off—and then regenerate its original state so it can signal again. The researchers used Anton to see how the “channel” turns off and then back on.

When the channel receives a signal from another cell, it activates, allowing potassium-ion flow and water molecules to enter its structure.

The water molecules force the filter closed.

When the signal stops, the channel inactivates and the water leaves.

The filter reopens, “resetting” the channel to activate again.

HOW ANTON HELPED

In the cell, the potassium channel can take as long as 10 to 20 seconds to reset its potassium filter. No computer currently on Earth can carry out such a long molecular dynamics simulation. But the University of Chicago researchers leveraged Anton to push their simulations to 20 microseconds. Even this relatively brief look was revealing, Roux says. “The system was stable for 20 microseconds in the pinched state,” he says. “That’s a long time in molecular dynamics. That was really shocking; we did not expect it.” But that didn’t mean the structure was static: The water molecules kept coming and going. Clearing the water molecules, and reopening the filter, was a “two steps forward, one step back” process, explaining the system’s slow recovery.

WHY IT’S IMPORTANT

The potassium channel helps create electrical signals in nerve and muscle cells. This process goes awry in some irregular heartbeat conditions. To work properly, every nerve or heart cell needs potassium channels that can activate, inactivate and then reset themselves to respond to the next signal.

In the journal *Nature*, Jared Ostmeyer, Benoît Roux and colleagues at the University of Chicago reported simulations on an Anton supercomputer, developed and provided by D. E. Shaw Research, hosted at PSC and funded by MMBioS, that revealed how the channel pinches off potassium movement.