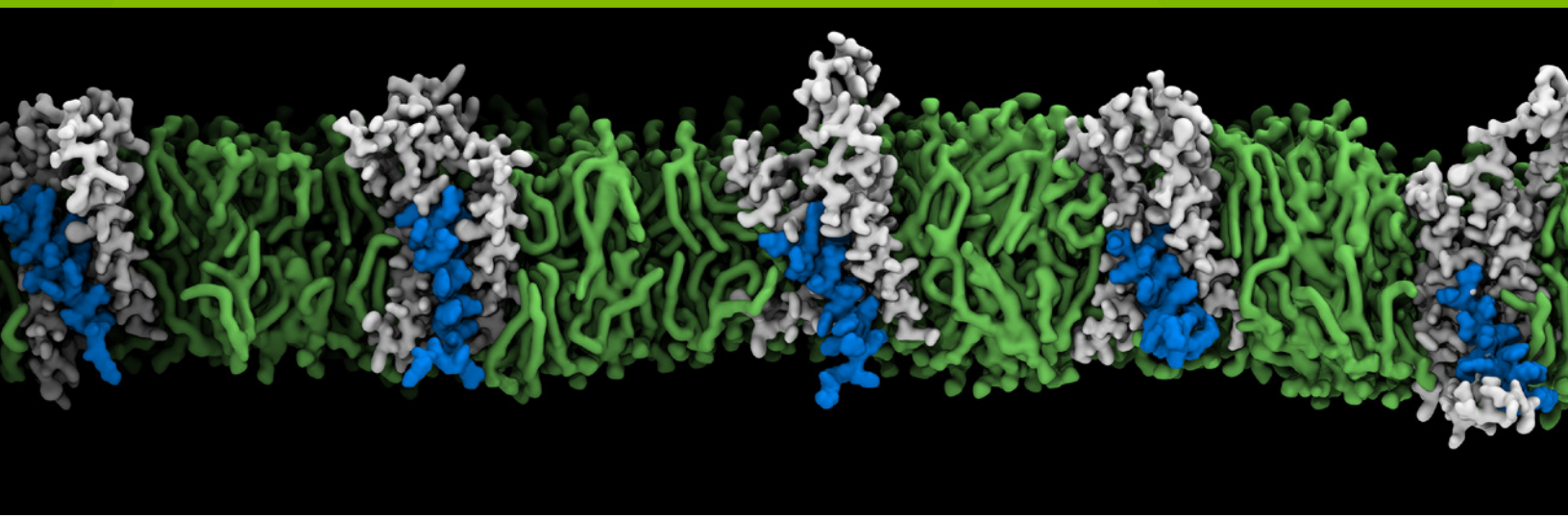
SUCCESS STORY | SCIENCE FOR LIFE LABORATORY

ACCELERATING THE FOREFRONT OF MEMBRANE TRANSPORT RESEARCH FOR DRUG DESIGN

NVIDIA® Tesla® GPU acceleration speeds up a range of molecular dynamics research running GROMACS simulations.



NVIDIA

Running GROMACS simulations on NVIDIA Tesla GPUs speeds up results by 4x, allowing researchers to publish higher accuracy research faster.

AT A GLANCE

CUSTOMER PROFILE

Customer: SciLifeLabs

Industry: Education/Research

Locations: Stockholm and Uppsala, Sweden

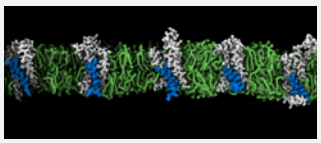
Size: Over 200 associated research groups

SUMMARY

- Leading Swedish research center offers technology and expertise to researchers.
- GROMACS is a leading molecular dynamics application offered at SciLifeLabs (among other places).
- Adding NVIDIA Tesla GPU acceleration shortens research cycles from one month to one week and allows more iterations for better results.
- One key project involves investigating voltage regulated ion channels to develop non-addictive painkillers.

REASONS FOR TESLA

1. Combines GPU accelerators and other technologies speed up scientific discoveries and insights
2. Massively parallel processing increase throughput for compute-intensive workloads
3. GROMACS can yield up to 4x performance on Tesla GPUs compared to non-accelerated systems.



Cover: Activation sequence of a voltage-sensing protein domain embedded in a membrane.

CUSTOMER PROFILE

Science for Life Laboratory (SciLifeLab) was founded in 2010 as a collaborative resource shared by four Swedish universities for researching molecular biosciences with a focus on health and environmental issues. Researchers from all of Sweden can access an infrastructure that includes state-of-the-art technologies to accelerate their projects. The center merges frontline technical expertise with advanced knowledge of translational medicine and molecular bioscience. Research conducted at SciLifeLab is used in the academic, industrial, healthcare, and government sectors.

One such project is an investigation being conducted by an intercontinental team into voltage-regulated ion channels that could find future application in the development of either non-addictive painkillers or more environment-friendly insecticides. This project relies on the GROMACS application developed by Stockholm University and the Royal Institute of Technology in Stockholm (KTH) to further epidemiological and pharmaceutical research.

BACKGROUND

The research group is studying the mechanisms behind various molecular phenomena that occur at human cellular membranes. A cell membrane acts as a barrier that isolates the interior of the cell from the outside world. Various molecules can be allowed passage through the membrane, thereby allowing a cell to communicate with its environment. For example, excitable cells such as neurons function by initiating and propagating electrical signals through the controlled transport of selected ions across the cellular membrane. The proteins involved in this cellular communications mechanism are referred to as a voltage-regulated ion channel.

As part of this project, the researchers are using GROMACS to run complex molecular dynamics simulations to accurately model the dynamical interplay between voltage-regulated ion channels and their environment.

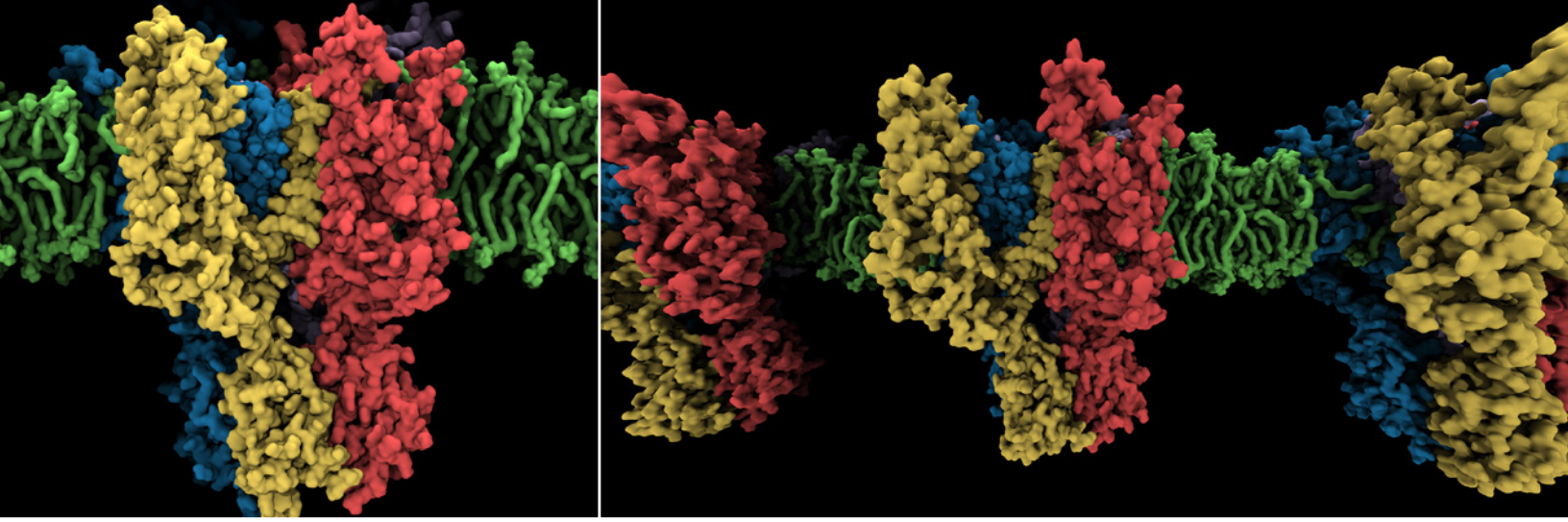


Figure 2: A voltage-regulated ion channel in its membrane environment viewed from the side.

Various drugs such as anesthetics, antiarrhythmic, and anti-epilepsy medications can work in voltage-regulated channels, provided those channels are well Achieving the required level of understanding requires many computationally expensive iterations.

Lucie Delemotte
Lead Researcher
SciLifeLab

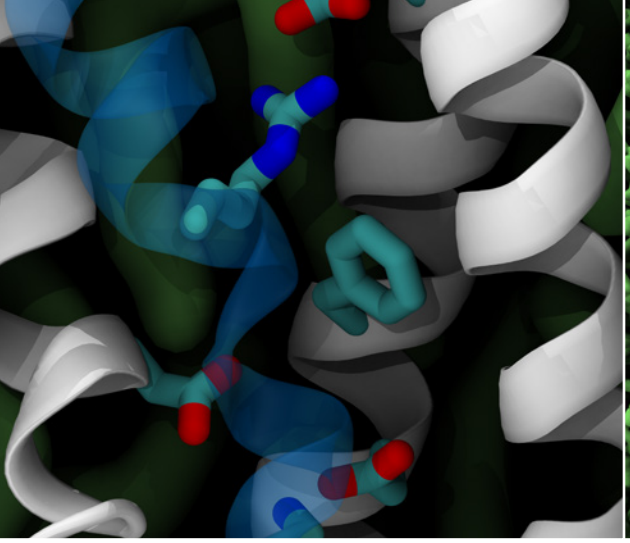
CHALLENGE

The key challenges for the researchers are the complexity of the molecules being studied and the many trial-and-error iterations required to calculate quantities of interest, such as the currents arising through the ion channel in response to electrical stimuli. Simulating each interaction is computationally intensive and takes over a month to run on a CPU-only system. The iterative approach makes it difficult to obtain results and publish research in a timely manner.

Traditional methods use experiments and a 'top-down' approach to model the behavior of a molecule. However, the researchers on this project are taking a reciprocal approach by using multiscale models to compute properties that can be directly compared with experimental (electrophysiology) measurements. This serves to validate the computational models used.

SOLUTION

GROMACS is a popular HPC application for molecular dynamics simulations. The GPU-accelerated version of GROMACS offloads heavy nonbonded force calculations to the GPU while concurrently using the CPU for bonded force calculations and lattice summation (PME). This optimization uses all-new algorithms that have been purpose-built and optimized for SIMD/streaming architectures, as well as support for parallel CPU/GPU calculations. It supports systems with single or multiple GPUs that have the CUDA development libraries installed.



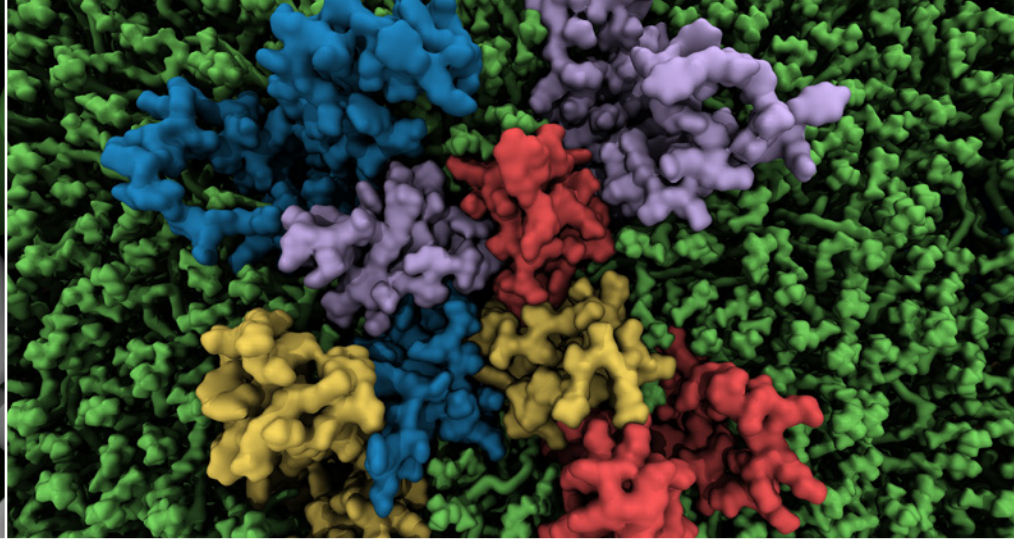


Figure 3: Zoom onto the molecular details of the voltage-sensing mechanism in a voltage-regulated ion channel.

Figure 4: A voltage-regulated ion channel in its membrane environment viewed from the top.

Running GROMACS simulations on Piz Daint at CSCS powered by the NVIDIA Tesla GPUs shortens our simulation time from one month to one week. We are also able to run more simulations for higher accuracy in less time. In this specific example, finding a non-addictive painkiller could revolutionize how we treat both acute and long-term pain. And that could help millions of people around the globe.

Lucie Delemotte
Lead Researcher
SciLifeLab

"Various drugs such as anesthetics, antiarrhythmic, and anti-epilepsy medications can target efficiently voltage-regulated channels, provided those channels are well understood," said Lucie Delemotte of KTH. "With GROMACS, we can mimic electrophysiological measurements by iteratively simulating the various molecular arrangements involved in the transport on the electrical signal."

NVIDIA Tesla GPUs are ideal for GROMACS workloads because they leverage massively parallel graphics processors to increase throughput for compute-intensive workloads.

RESULTS

The highly iterative nature of fitting the parameters of the kinetic models used to simulate the electrical current curves and running compute-heavy simulations for each consumes both time and resources. Slower simulations mean fewer iterations, which can mean lower accuracy in the parameters and the model outcome and therefore in the understanding of the mechanism being studied.

Adding GPU acceleration provides a significant performance boost. Faster simulations allow more trials within a given time period, which boosts the efficacy of the research.

"Running GROMACS simulations on Piz Daint at CSCS powered by the NVIDIA Tesla GPUs shortens our simulation time from one month to one week," concluded Delemotte. "We are also able to run more simulations, thereby ensuring that we indeed found the optimum description of the mechanisms of interest for achieving our goals. When we started this project four years ago, this accomplishment seems overambitious but we met our objectives, thanks to GROMACS and GPU computing."

"In this specific example, finding a non-addictive painkiller could revolutionize how we treat both acute and long-term pain. And that could help millions of people around the globe."

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