Research software development

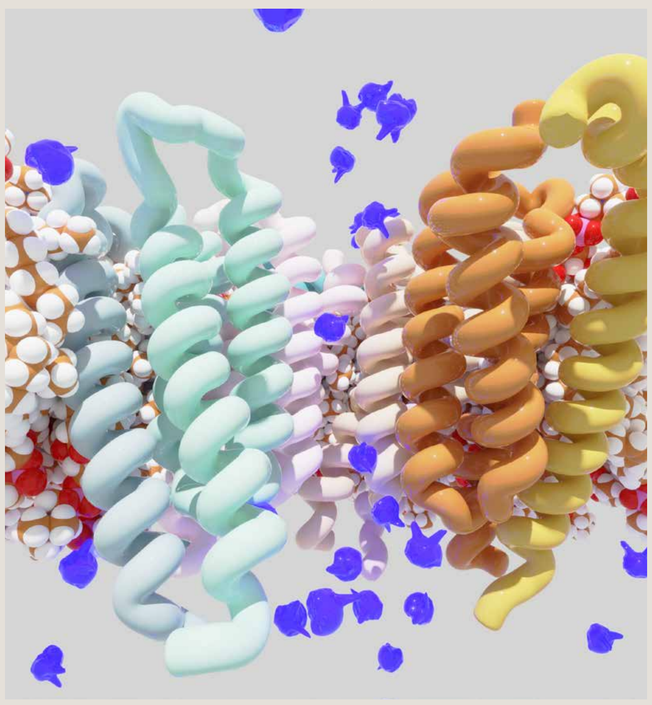
PDC develops world-leading scientific research software capable of leveraging modern supercomputers

GROMACS

FAST. FLEXIBLE. FREE.

Molecular Dynamics (MD)

Simulating molecules and their interactions is a cornerstone in biomolecular and materials science research. Researchers from KTH and Stockholm University head the development of GROMACS, the leading molecular dynamics simulation code, which is used worldwide.



This illustration is from a study using MD simulations with GROMACS to investigate how nicotinic acetylcholine receptors work in the human body. These proteins help cations to pass through the postsynaptic membrane in the brain, which leads to signals being propagated through our nervous systems. The precise identification of critical protein residues that govern protein function through MD simulations holds significant promise for guiding the design of medications that could be used to treat anxiety and depression.

NEKO

Computational Fluid Dynamics (CFD)

It is becoming challenging to adapt older CFD code for new supercomputers which contain graphics processing units (GPUs) and not just CPUs. Researchers at KTH/PDC develop Neko to run high-fidelity fluid simulations on “accelerated” GPU-based systems.

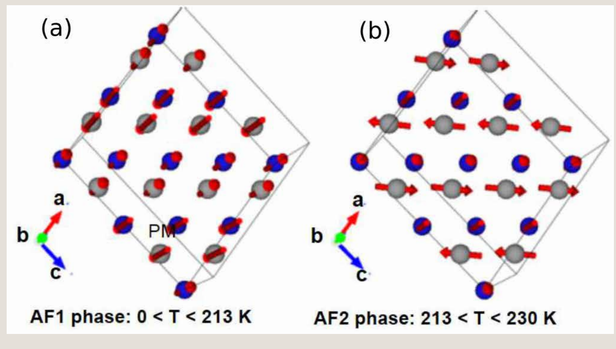
Neko is, for example, used to perform large-scale numerical simulations for research and development in sustainable transport. The image is from a study on Flettner rotors. They are rotating cylinders that spin around their long axes as air passes across them. They were invented as rotor sails for ships about a hundred years ago and are now being studied as a clean and efficient method of propulsion to reduce fossil fuel usage. When developing rotor sails, it is essential to understand how air flows around a Flettner rotor and how that flow of air interacts with potentially turbulent air close to the surface of the rotor (known as a turbulent boundary layer). The image is from a simulation looking down at the top of a Flettner rotor (the white circle in the centre) in a turbulent boundary layer. The colours indicate the velocity of the airflow with violet representing low speeds, white for medium speeds, and orange for high speeds.

UppASD

Atomistic Spin Dynamics

UppASD has been developed by researchers at Uppsala University and KTH to simulate magnetisation dynamics on an atomic level. This makes it possible to model how the magnetic moments and behaviour of particular materials change under different conditions.

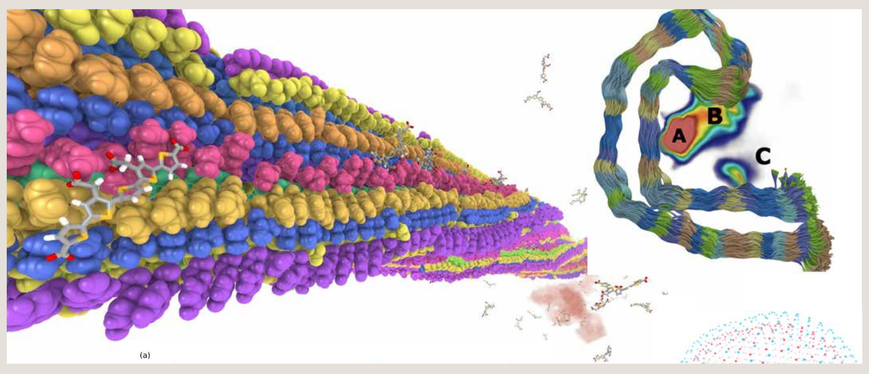
Antiferromagnetic materials – such as cupric oxide, CuO – are substances that do not have an overall external magnetic moment (although ions within the material act as tiny individual magnets as a result of how the electrons spin). These substances can therefore be used as insulators in electronic components, for example, for data storage. It is important to be able to predict how these materials will behave magnetically at different temperatures and under different conditions when developing new products. The figure shows spin configurations of two competing phases that occur in CuO at different temperatures: (a) AF1 and (b) AF2. The red arrows indicate the spin polarisation of the blue and grey CuO atoms. When CuO is in the AF2 phase, the system has both magnetic and ferroelectric properties, which means the magnetic ordering could be controlled by applying an electric field. Such multiferroic materials have potential for use in future energy-efficient data storage.



VELOXCHEM

Quantum Chemistry Molecular Modelling

The Veloxchem quantum chemistry software is developed by KTH/PDC researchers to make it easier for computational chemists to calculate molecular properties and simulate a variety of spectroscopies.



Veloxchem is, for example, being used in research aimed at developing ligands (molecules that bind to receptors in the human body) for early-stage detection of Alzheimer’s disease. Molecular dynamics simulations are performed with GROMACS to find sites where ligands could bind to amyloid fibrils. (The fibrils are a type of plaque that develops in the brains of people with Alzheimer’s, so being able to detect the fibrils can help with diagnosing Alzheimer’s early on.) Quantum mechanical spectrum simulations with VeloxChem are then used to check if particular ligands do bind to the proposed sites on the fibrils by comparing with photophysical experiments. Once suitable ligands are found, they can be used with brain imaging to check if patients are developing fibrils.

PDC Center for High Performance Computing

NAISS