# Software at PDC

PDC has software installed for modelling and simulation, along with compilers and other software tools - these are available to all researchers using our facilities. Some examples of the available software are listed below. Our Support group and Application Experts can also help you with compiling, installing and optimizing software. In addition PDC has licenses available for some commercial software, though usually research groups need to pay the license fee to use such software. For more information, contact PDC Support or see

https://www.pdc.kth.se/software

Electronic Structure

- Dalton
- Gaussian
- Jaguar
- NWChem
- Quantum Espresso
- VASP
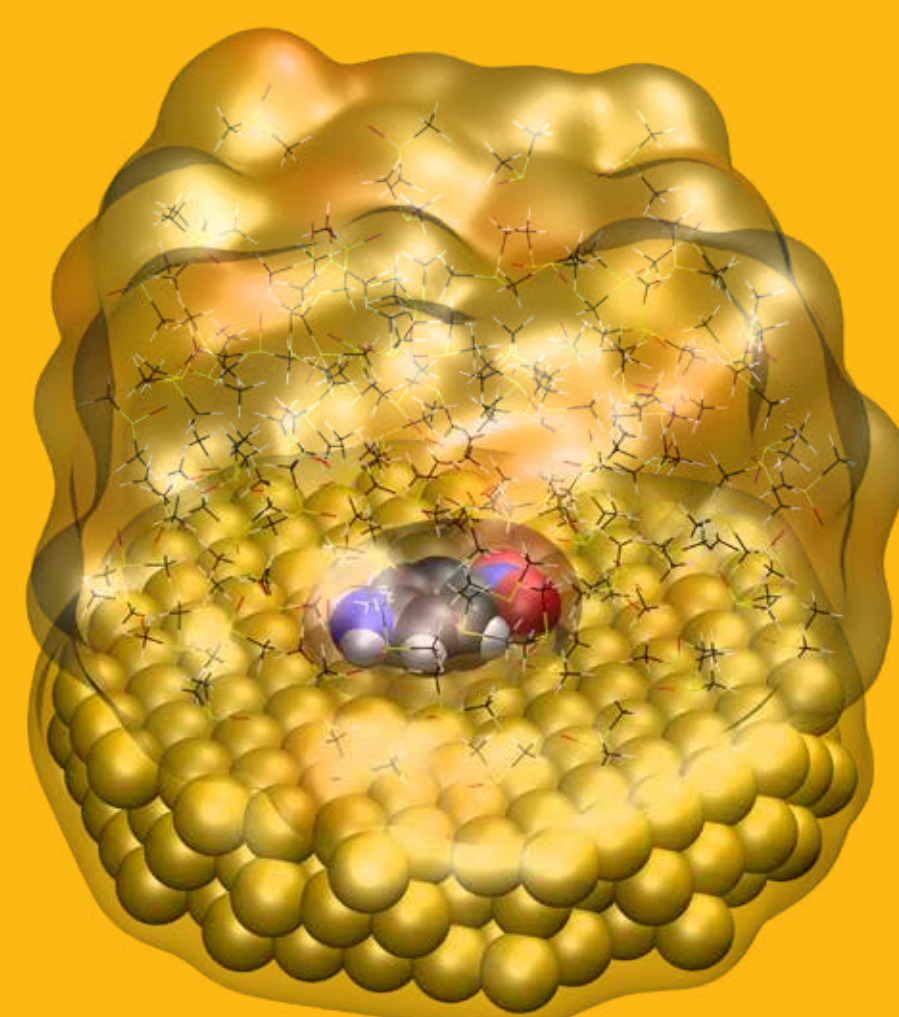
Mathieu Linares (Division of Theoretical Chemistry and Biology, KTH) used Dalton to compute the UV/VIS and X-ray spectra of a PNA molecule adsorbed on an Au(111) surface in a solvent of dimethyl sulfoxide molecules. The structure for the image was generated using the GROMACS MD package.

Bioinformatics
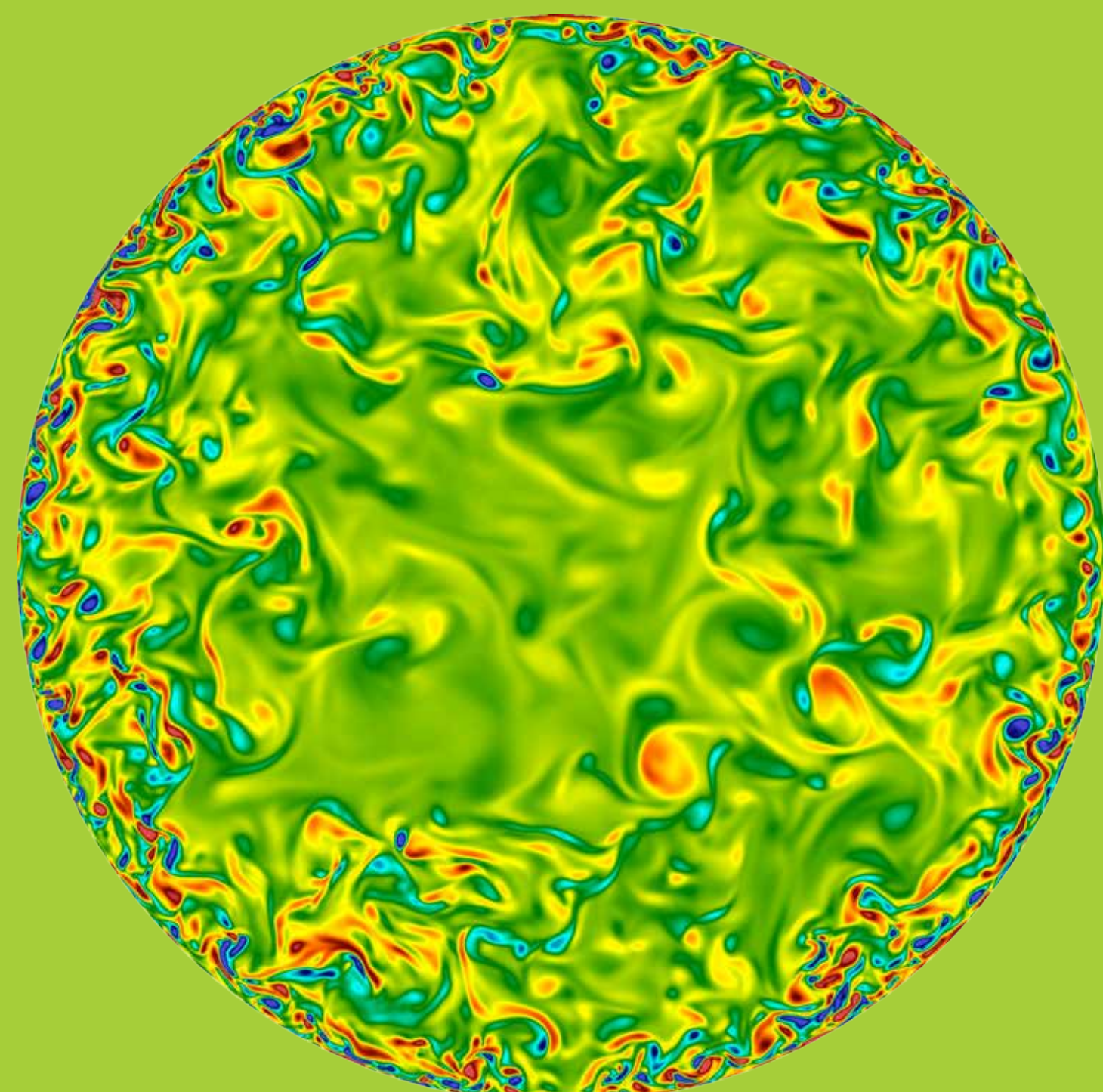
- Allpaths-LG
- Blast
- Falcon
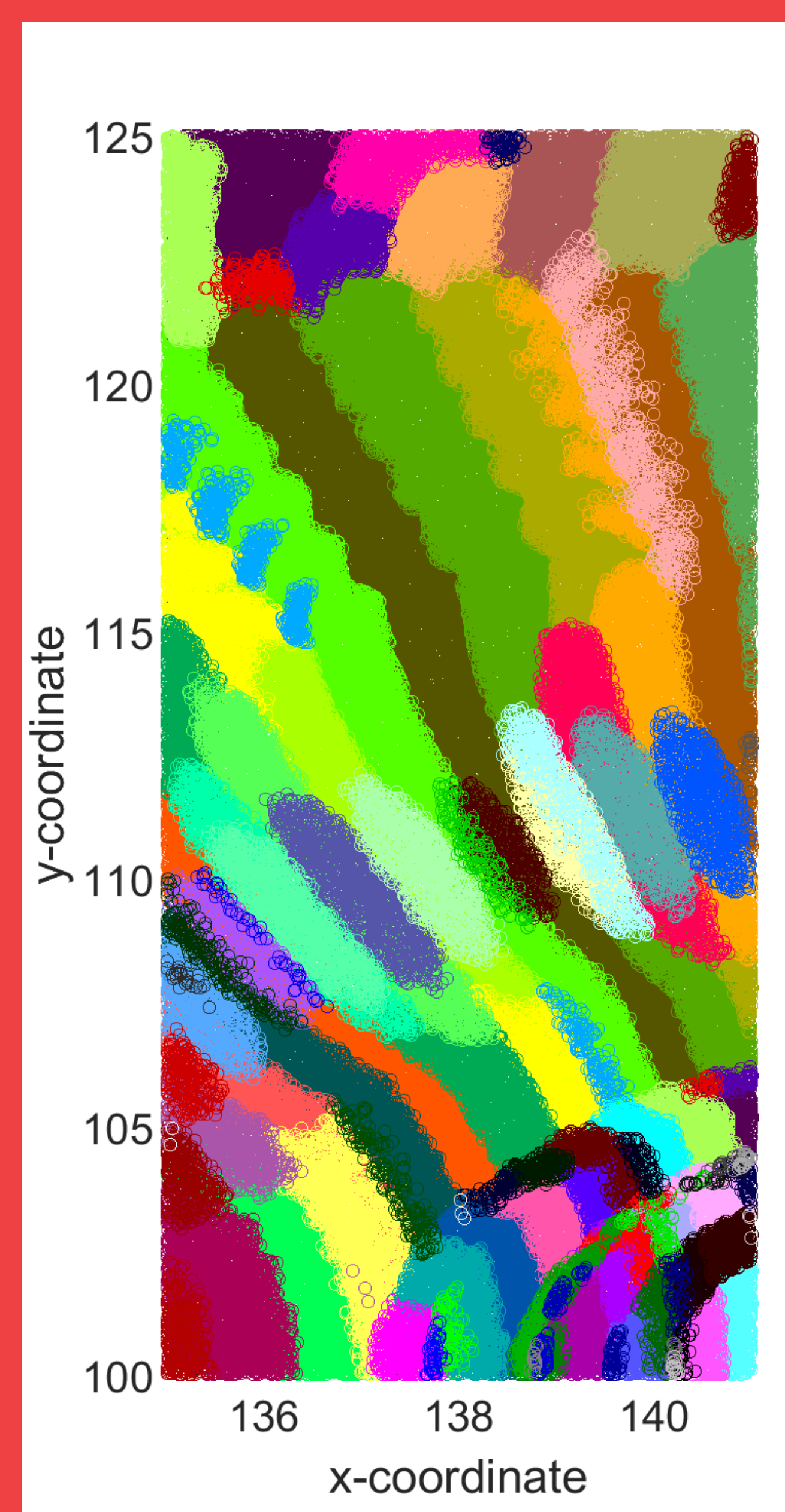- PhyloBayes
- Ray
- SAMtools

Physics and Engineering

- Nek5000
- StarCCM+
- OpenFOAM
- PowerFLOW
- ANSYS (Fluent, CFX)
- Comsol
- Abaqus
- LS-DYNA

Philipp Schlatter (Department of Mechanics, KTH) used Nek5000 to simulate a cross-section of a long pipe with fluid flowing through it. The resulting image demonstrates that turbulent flow produces vortices, particularly around the edges of the pipe.

Tools and compilers at PDC

- Intel compiler suite
- PGI compiler suite
- DDT debugger and MAP profiler
- Open-source software

Machine Learning

- TensorFlow
- PyTorch
- Keras
- MatConvNet

Mathematics

- MATLAB
- R
- SageMath
- Mathematica
- CPLEX

Sahar Imtiaz (Division of Information Science and Engineering, KTH) created this image using MATLAB. It shows the distribution of resources in a wireless communication system with a single transmitter serving a single receiver. Each of the circles represents the position of a receiver, and the colour denotes a unique combination of resources allocated for serving the receiver at the given position. In all, there are 137 unique combinations of system resources that maximize the throughput of the wireless communication system with a single transmitter serving a single receiver.

Molecular Dynamics

- GROMACS
- NAMD
- LAMMPS
- Amber
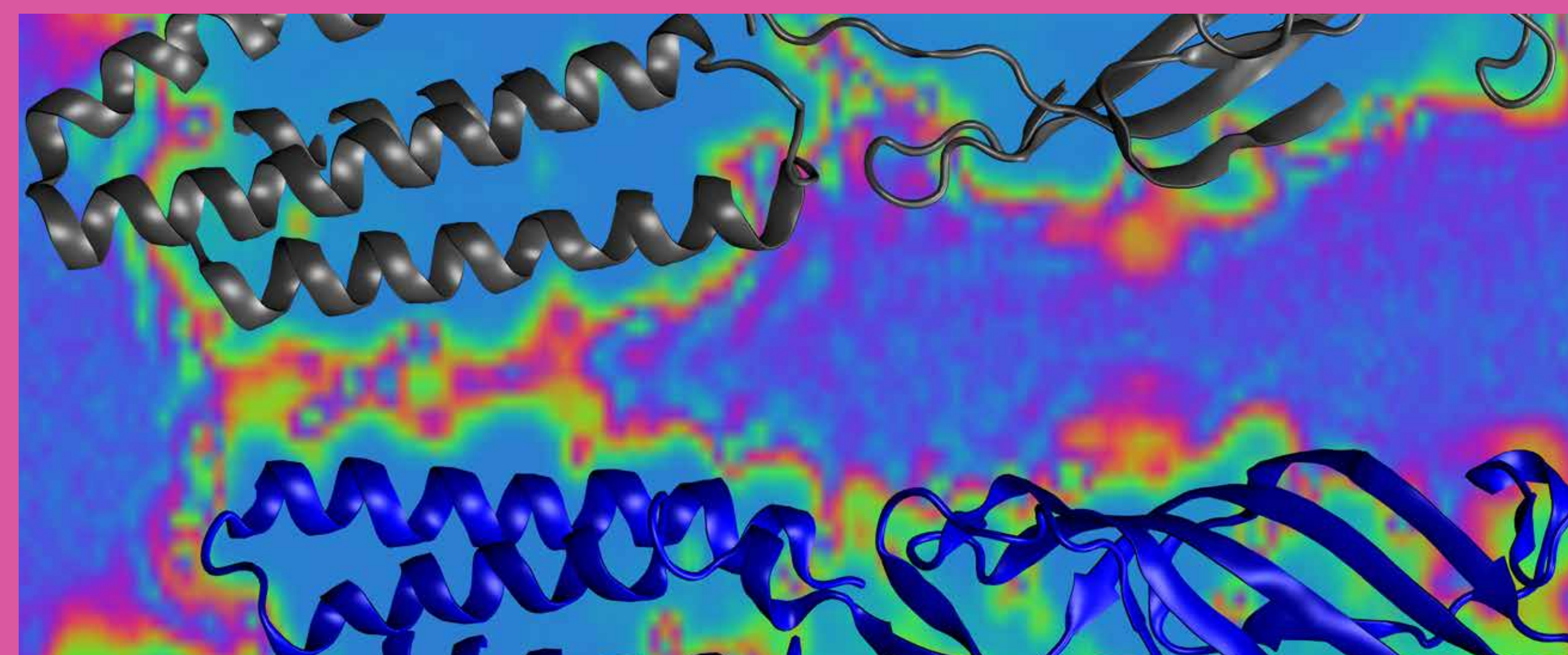
This image of a gloeobacter ligand-gated ion channel (GLIC) protein was generated from simulations using GROMACS by Iman Pouya (Department of Physics, KTH).

Access QR code or visit www.pdc.kth.se for more information.

PDC Center for High Performance Computing SNIC