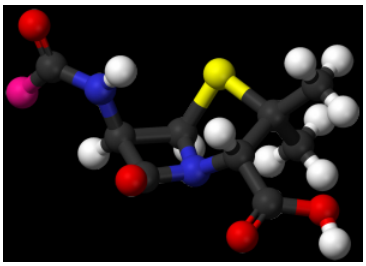
Molecular Dynamics



Penicillin

StreamHPC has carried out several successful parallel-computing projects in molecular dynamics since 2012. Below are a few examples of our work in bioinformatics, chemistry and meteorology.

Gromacs

GROMACS is one of the fastest molecular dynamics software packages on the market. To **broaden the user base** that can benefit from the processing power of modern GPUs, we ported GROMACS **from CUDA to OpenCL** and further optimised the code for use with AMD FirePro accelerators. The resulting performance is on a par with that of the original CUDA code but without the restriction of being bound to a specific parallel computing hardware. GROMACS is used world-wide by over 5000 research centers, from simulating molecular docking to examining the hydrogen bonds in a falling water drop. Read more...

STANFORD UNIVERSITY
DEPARTMENT OF CHEMISTRY

For the university of Stanford, we **further optimised** a part of TeraChem, a general purpose quantum chemistry software designed to run on NVIDIA GPU architectures. Our work resulted in adding an **extra 70% performance** to the already optimised CUDA code.

MANCHESTER 1824
The University of Manchester

For the University of Manchester, we developed a high-performance implementation of the UNIFAC group contribution model for their research on atmospheric aerosol particles. Where an OpenMP implementation of the original single-threaded code got the run time down from 32 to about 10 seconds on a quad-core CPU, we eventually brought it down to 0.062 seconds using OpenCL on a Xeon Phi accelerator ? a **speedup of 160x over OpenMP**. Read more...