BBB Seminar (BMED380)

SCAN ME

Thursday, June 5. 14:30 at the BBB, **NB! Auditorium in AHH**

Biomolecular simulations in the age of exascale computing

Andreas Goetz
San Diego Supercomputer Center, University of California, San Diego, USA

This talk will give a perspective on challenges, opportunities, and some recent developments for biomolecular simulations within the context of the rapidly evolving computer hardware landscape. With the end of Moore's law, performance gains come from a combination of software, algorithms, and hardware. Streamlined hardware with many simplified processor cores running in parallel for instance can lead to large efficiency gains for algorithms that can exploit this parallelism. Domain specialization is another way to increase efficiency, where hardware is customized to a specific application domain. This results in heterogeneous compute architectures, with a combination of central processing units, graphics processing units (GPUs), and other hardware such as accelerators for artificial intelligence (AI) workloads.

As an example I will discuss developments in Amber, a biomolecular simulations software that is used by thousands of scientists in academia, national labs, and industry for computational drug design and related research. Amber is well known for its high-performance molecular dynamics (MD) program, which features a very efficient CUDA implementation for Nvidia graphics processing units (GPUs) that has been continuously optimized since its initial release over a decade ago. This enables fast MD simulations with millions of atoms both on datacenter and consumer grade Nvidia hardware. Recently, a HIP/ROCm implementation has become available to enable Amber MD simulations on AMD devices and a SYCL implementation for Intel GPUs is under development.

I will also discuss our recent efforts in developing QUICK, an open-source *ab initio* quantum chemistry program that runs on GPUs. QUICK enables quantum mechanical / molecular mechanical (QM/MM) molecular dynamics simulations in combination with Amber. I will further discuss the rapid progress in AI and machine learning (ML) that has driven GPU and specialized AI processor development, and how AMBER can employ ML-corrected semiempirical QM/MM-ΔML methods to speed up costly QM/MM simulations.

Chairperson: Knut Teigen, Department of Biomedicine