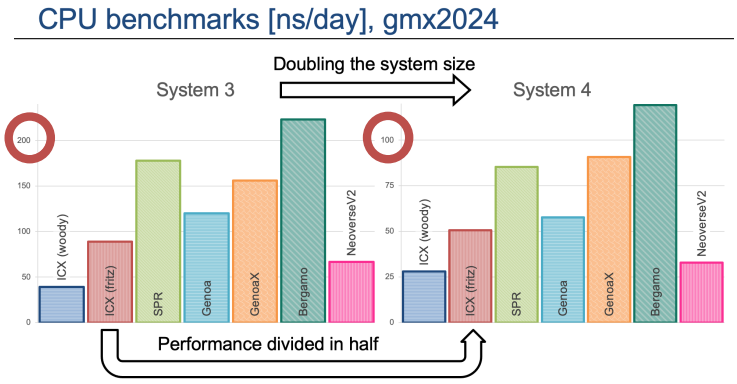
Performance optimization of GROMACS on modern Hardware

Anna Kahler, Thomas Zeiser, Gerhard Wellein

Erlangen National High Performance Computing Center
Friedrich-Alexander-Universität Erlangen-Nürnberg

The MD simulation code GROMACS runs out of the box on CPUs and has been able to offload time-consuming calculations of electrostatics that use the Particle Mesh Ewald approach to GPU since version 2018. In the past years, GROMACS developers have added GPU offloading for bonded interactions and for the calculation of updates and constraints. With these code changes, the following questions may arise: Which hardware yields the best performance results? What are the optimized runtime parameters? How does the performance change across different hardware and software versions?



To find answers, a variety of benchmarks is run on different hardware architectures including CPUs and GPUs. The results not only give insights into scaling behavior regarding system size or show performance increases with the most recent program version or on the newest GPU but also reveal a need to assess runtime parameters for each project individually and based on the used hardware.