Optimizing energy consumption in classical and quantum molecular dynamics calculations

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Computational Material Science appears to be an essential part of modern high-performance workloads – it requires usage of complicated and precise atomistic and quantum models to solve its problems. The gradual increase in size and complexity of used molecular dynamics or ab-initio models results in substantial growth in demanding computational performance. Furthermore, this trend leads to significant rise of supercomputer total energy consumption and its capability to dissipate heat, thus becoming another scalability barrier along with high cost of supercomputing hardware.

In the first part of our speech, we will discuss the GPU-accelerated molecular dynamics and how the advancement of modern GPU applies to their performance in MD-code LAMMPS (USER-CUDA and GPU packages) and their hardware-monitored energy consumption. We will show the existence of energy-effective GPU frequency modes.

In the second part of our speech, we will discuss the choice of supercomputing hardware for effective and cost-effective quantum ab-initio simulations – in particular, one of the most popular software of such kind, VASP. We will show how the balance between computational power (e.g. cores) and memory performance (number of memory channels, cache size) of high performance system impacts on the speed of solution of ab-initio problem and energy consumption.