Supercomputer architectures and acceleration of molecular dynamics calculations

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Molecular dynamics (MD) methods are among the most computationally demanding numerical tools for materials science, chemistry, biology and other fields. The computational complexity of MD calculations is determined by the number of atoms that should be considered in the model and by the potential or forcefield that should capture the essential traits of interatomic interaction. The development of supercomputers is the major reason why the MD calculations can be applied to the growing list of real-life problems.

However the efficient acceleration of MD calculations on the particular supercomputer architecture is not always easy to achieve. This is the case of hybrid architectures based on GPU accelerators. In this talk I will present the history of the development of GPU-aware classical MD algorithms and their current efficiency. Their advantages and disadvantages with respect to CPU algorithms will be discussed.

The MPI-based internode communication is another bottleneck of MD codes. The comparison of different architectures with respect to the strong scaling of classical MD models will be presented for the cases of different topology of interconnect (fat-tree or torus) and up to 10 PFlops of the total peak performance of the nodes. MPI communications are very pronounced in ab initio MD parallel algorithms, which strong scaling will be discussed as well.