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Scalable polarizable molecular dynamics using Tinker-HP

Jean-Philip Piquemal

Sorbonne Université, Laboratoire de Chimie Théorique, U;R7616, 75005 Paris France
Institut Universitaire de France, 75005, Paris, France
Email: jean-philip.piquemal@sorbonne.universite.fr

Tinker-HP [1] (http://www.ip2ct.upmc.fr/tinkerHP) is a CPU based, double precision, massively parallel package dedicated to long polarizable molecular dynamics simulations and to polarizable QM/MM. Tinker-HP is an evolution of the popular Tinker package [2] (http://dasher.wst1.edu/tinker) that conserves its simplicity of use but brings new capabilities allowing performing very long molecular dynamics simulations on modern computers that use thousands of cores. The Tinker-HP approach offers various strategies using domain decomposition techniques for periodic boundary conditions in the framework of the (N)log(N) Smooth Particle Mesh Ewald. Tinker-HP proposes a high performance scalable computing environment for polarizable force fields giving access to large systems up to millions of atoms. I will present the performances and scalability of the software in the context of the AMOEBA force field. Various benchmarks and examples on bimolecular systems will be provided on several architectures. As the present implementation is clearly devoted to petascale applications, the applicability of such an approach to future exascale machines will be exposed and future directions of Tinker-HP discussed in the framework of our ERG SYG EMC2 project. New results towards large scale QM/MM hybrid simulation coupling polarizable force fields and Density Functional Theory (DFT) [3] will be presented.

References

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