MASSIVELY PARALLEL COUPLED CLUSTER THEORY ALGORITHMS FOR MATERIAL SCIENCE

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Abstract

Many of the most important challenges our society has to face in the next decades are related to materials science. Computer simulations are expected to contribute significantly to the development and understanding of materials that exhibit specific properties to fulfil key tasks in more efficient and novel devices as well as chemical processes. The properties of most materials arise largely from the quantum mechanics of their constituent electrons under the influence of the electric field of the nuclei. Consequently, the accurate solution of the underlying many-electron Schrödinger equation is at the heart of ab initio calculations in materials science.

A promising class of approximations widely used in quantum chemistry to solve the many-electron Schrödinger equation is the so-called coupled-cluster family of methods. These methods achieve for a large class of systems a high accuracy at a comparably moderate cost. Here, we report results of state-of-the-art simulations employing high performance computing resources to produce reliable benchmark results of molecules and surfaces containing more than 50 atoms. These benchmark results are needed to advance computationally more efficient but less accurate theories that can be improved by adjusting parameters and will ultimately be needed to model real materials in their full complexity.

Computational materials science simulations can be useful in exploring the performance of computational infrastructures and algorithms. Memory and computational bounds appear often in a challenging interplay, which makes their investigation through sophisticated parallel algorithms necessary. In this poster we present an implementation of a widely-used theory called `CCSD(T)`. This theory achieves a high degree of accuracy for thermochemical systems at the price of a moderately high computational cost. This implementation has been specifically tailored to efficiently calculate a large number of electrons. Our novel algorithm is based on the use of asynchronous MPI and reaches a high performance across a large numbers of cores. The usage of HPC resources is of significant importance for our ab initio simulations on the level of CCSD(T) theory.

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