The Divide-Expand-Consolidate Scheme for Massively-Parallel Molecular Science Computations

Dmytro Bykov, Pablo Baudin, Janus Eriksen, Patrick Ettenhuber, Thomas Kjaergaard, Kasper Kristensen, Filip Pawlowski, Yang Min Wang and Poul Jørgensen

The Divide-Expand-Consolidate (DEC) scheme can be applied to evaluate molecular energy and properties in a linear-scaling and embarrassingly parallel manner using a set of local Hartree-Fock molecular orbitals. The essence of the method lies in the fact that all the manipulation of the intermediate four-dimensional quantities are carried out independently within small local orbital fragment spaces. The sizes of the orbital fragment spaces are determined in a black-box manner to ensure that the error in the DEC implementation is proportional to a single input threshold, denoted as the fragment optimization threshold (FOT). The scaling behavior, performance and benchmark studies as well as series of illustrative calculations prove the DEC method to be highly effective tool for approaching large molecular systems.