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High-efficiency parallelization of programs, implementing the Hartree-Fock method, the density functional theory, and the configuration interaction method

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Abstract. It is shown that the modified method of Fock matrix calculation with data compression, using the stored integrals, scales linearly with respect to the number of basis functions for large molecular systems. This method leads to the development of the high-efficient parallel algorithms of the conventional and semi-direct Hartree-Fock and the density functional theory (TDF) methods. The main approaches are formulated for the parallelization of the configuration interaction (CI) method with the configurations selection, in which the matrix elements are calculated by using the Slater rules. The efficiency and the application of the proposed approaches is demonstrated.

Keywords: distributed computations, parallel computations, Hartree-Fock method, Kohn-Sham method, configuration interaction method

MSC numbers: 65Yxx, 65Y05, 65Y10, 92Exx, 92E10, 92C40

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