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First steps in implementing the RI-HF algorithm for electronic structure calculations

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The Hartree-Fock (HF) method is one of the most important methods of electronic structure theory. So there is interest in this algorithm, for example, within the framework of a future software ecosystem for high-precision multi-scale *ab initio* relativistic quantum modeling of atoms, molecules, and materials (part of the BUFO program [1]). But the conventional sequential program implementation of the HF algorithm is too slow and memory-intensive since the evaluation and storage of four-center molecular integrals are needed in HF to obtain the matrix elements of the Coulomb and exchange operators. Therefore, it is considered to be a key bottleneck of the algorithm. Several methods have been designed to speed up this part of the algorithm, one of which is known as resolution of identity approximation (RI) [2]. This method allows to skip evaluation and storage of four-center molecular integrals to vector-matrix operations with two- and three-center integrals and storage of them. The latter can be significantly or sometimes completely organized in RAM of several CPUs or GPUs, unlike four-center integrals. This organization gives a large performance gain because vector-matrix operations to obtain the matrix elements of the Coulomb and exchange operators can be efficiently done in parallel. Thus, if we want to obtain a highly efficient version of the HF algorithm, the most promising option is to develop the RI-HF version. It is done using the libcint library for calculating integrals [3] and using vector-matrix multiplications [4]. The results were compared with those in the ORCA program package [5].

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