Cholesky Decomposition in Quantum Chemistry: A summary of the current status

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Abstract

This lecture is a brief presentation of the development of the Cholesky decomposition of two-electron integrals [1] and the implementation of the technique in contemporary ab initio methods as it stands today. The presentation will discuss the use of the method in standard wave function and density functional theory models, the development and implementation of the associated analytic gradients, and benchmark results with respect to accuracy and overall timings [2]. The lecture will present evidence why the CD technology is the optimal and most effective way to eliminate the need of precomputed RI auxiliary basis sets.

[1] Simplifications in the generation and transformation of two-electron integrals in molecular calculations, N. H. F Beebe and J. Linderberg, *Int. J. of Quantum Chem.*, 12:683-705, 1977, DOI:10.1002/qua.560120408

[2] Cholesky decomposition techniques in electronic structure theory, F. Aquilante, L. Boman, J. Boström, H. Koch, R. Lindh, A. Sánches de Marás and T. B. Pedersen, in Linear-Scaling Techniques in Computational Chemistry and Physics, Eds. R. Zalesny, P. G. G. Mezy, M. G. G. Papadopoulos and J. Leszczynski, vol. 13, chapt. 13, pp. 301-343, 2011. DOI: 10.1007/978-90-481-2853-2