The history of Cholesky Decomposition in QC from 1977 until today

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Abstract
In this brief presentation we will tell the story of how the Cholesky Decomposition (CD) (a method designed by Andrés-Louis Cholesky, Fig. 1, in the late 19th century[1]) of the electron-repulsion integrals (ERIs), used in quantum chemical (QC) calculations, has not until recently been appreciated and used to its full capacity. Whilst the initial paper[2] (Figs. 2 and 3 depicts the authors) highlighted *efficiency* in transformation from atomic to a molecular basis of the ERIs, the recent newer understanding[3] of the CD additionally include *accuracy* of auxiliary basis sets as a further specific characteristics of the approach. Furthermore, proper implementation of CD facilitates *optimal* presceening in the ERI generating step. In this presentation we will highlight these aspects and present the current status and implementation of CD in QC. Benchmark results will be presented with respect to accuracy in computing reaction energies, excitation energies and non-covalent intermolecular interaction energies. Efficiency improvements with respect to CPU demands in computing analytic CD gradients for the HF, pure and hybrid DFT, and MP2 methods will be presented. CD-CASSCF gradients will be discussed.

References:
[1] Cdt. Benoît, "Note sur une méthode de résolution des équations normales provenant de l'application de la méthode des moindres carrés à un système d'équations linéaires en nombre inférieur à celui des inconnues, (Procédé du Commandant Cholesky)", Bulletin Géodésique, **1924**, *2*, 67-77.
[2] N. H. F. Beebe, J. Linderberg,"Simplifications in the Generation and Transformation of Two-Electron Integrals in Molecular Calculations", *Int. J Quantum Chem.*, **1977**, *12*, 683-705.
[3] F. Aquilante, L. Boman, J. Boström, H. Koch, R. Lindh, A. Sánchez de Merás, T. B. Pedersen, "Cholesky Decomposition Techniques in Electronic Structure Theory", in *Linear-Scaling Techniques in Computational Chemistry and Physics. Methods and Applications*, Eds.: R. Zalesny, M. G. Papadopoulos, P. G. Leszczynski, Springer, **2011**, Vol. 13, Chapter 13, pp 301-343.

Fig. 1 Andrés-Louis Cholesky, the inventor of the Cholesky decomposition method.

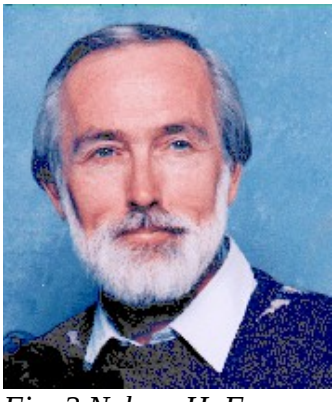
Fig. 2 Nelson H. F Beebe, coauthor of reference 2.


Fig. 3 Jan Linderberg, coauthor of reference 2.