Recent advances in the use of Cholesky decomposition within electron-correlated calculations of energy and properties

Jürgen Gauss

Department Chemie, Johannes Gutenberg-Universität Mainz,
Duesbergweg 10-14, D-55128 Mainz, Germany

In this presentation, recent advances in the use of Cholesky decomposed two-electron integrals within electron-correlated quantum-chemical calculations are discussed. In particular, a Cholesky decomposition based implementation of a quadratically convergent complete active-space self-consistent field (CASSCF) scheme and second-order Møller-Plesset perturbation theory (MP2) implementations for the computation of magnetic properties (NMR chemical shifts and magnetizabilities) using Cholesky decomposed unperturbed and perturbed two-electron integrals are presented. The computational efficiency of these implementations is demonstrated by large-scale applications involving up to 100 atoms and more than 1000 basis functions.