Coupled-cluster methods in single precision

Pavel Pokhilko[1] , Anna Krylov[1] , Evgeny Epifanovsky[2]

1. Department of Chemistry, University of Southern California, Los Angeles, CA, United States.
2. Q-Chem, Inc., Pleasanton, CA, United States.

Libtensor library for tensor contractions has been augmented by single precision operations. Application on CCSD shows speed up of a factor of 2 on various CPU architectures. We have implemented several variants of CCSD in single precision, differing by storing or re-computing of integrals, including resolution-of-identity and Cholesky decompositions, and by recovering of numerical accuracy. The results show that single precision CCSD iterations do not introduce a significant numerical error and the later can corrected by just a few additional iterations in double precision. Even on the systems with problematic convergence, this procedure reduces total wall times of calculations, providing the same numerical accuracy as full double precision calculation.