Artificial intelligence for electronic structure: Automated parallel implementations of configuration-interaction, coupled-cluster, and many-body perturbation theories

So Hirata

Pacific Northwest National Laboratory

K8-91, P.O.Box 999, Richland, WA 99352

Many-electron theory offers a variety of converging approximations to tackle chemical problems. However, such studies are often deterred not only by limited computational resources but to a greater extent by the immense complexity of the process of deriving the working equations and implementing efficient programs of the approximations, which can even take man-years of efforts. We present an algebraic and symbolic manipulation program that abstracts and automates altogether the derivation and parallel implementations of second-quantized models of many-electron theory and its applications to parallel implementations of CI up to CISDTQ, CC up to CCSDTQ, non-canonical MBPT up to fourth order, EOM-CC up to EOM-CCSDTQ, and CC lambda equation up to CCSDTQ. These computer-generated programs fully take advantage of spin, spatial, and index permutation symmetry, adjust memory usage by tiling algorithm, and balance parallel workload dynamically, and can compete with carefully hand-coded programs in performance. Applications of some highly correlated (relativistic) methods derived and implemented by this automated system to second- through fifth-row diatomic and triatomic hydrides (with Drs T. Yanai, W. A. de Jong, T. Nakajima, and K. Hirao) and cluster and solvation chemistry (with Drs. H. Sekino, S. Xantheas, and M. Dupuis) will also be addressed.

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