Development of MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculations for massively parallel multicore supercomputers

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Second-order Møller–Plesset perturbation theory (MP2) is the simplest but robust electron correlation method to account for the non-covalent interactions that play important roles in the chemical phenomena of nano and biological molecules. However, the computational cost of MP2 calculations scales $O(N^5)$ with respect to the size of molecules (N), and practical applications are limited to molecules of moderate size. To make the MP2 calculations applicable to the large nano and biological molecules, development of efficient computational techniques is desired.

We have developed a MPI/OpenMP hybrid parallel algorithm of resolution of identity MP2 (RI-MP2) calculations suitable for the massively parallel calculations on muticore supercomputers such as K computer by improving the previous algorithm [1] developed by authors. In the previous algorithm, the occupied orbital pairs are distributed to processors for the calculation of four-center two-electron integrals. However, the number of occupied orbital pairs is small, and this makes the load balancing problems in the cases of the massively parallel computations. We have changed to use the virtual orbital and its pair for the MPI parallel task distribution in order to use more large number of CPU cores with the efficient load balancing. Generally, the number of virtual orbitals is more than four times larger than the number of occupied orbitals, and the load valancing is considerably improved from the original algorithm. Computationally demanding tasks inside of MPI parallelized loops are mainly matrix-matrix multiplications and efficiently parallelized by OpenMP version of optimized BLAS libraries such as Intel MKL and AMD ACML. The algorithm is also designed for the massively parallel calculations by avoiding the I/O overheads and reducing network communication overheads. We have implemented the parallel RI-MP2 algorithm into NTChem quantum chemistry software. The new implementation has been supplied as library software on K computer.

Using the new MPI/OpenMP hybrid parallel RI-MP2 codes in NTChem, MP2 calculations of large molecules having up to 300 atoms and 7000 atomic orbitals can be performed with high parallel performance and in modest times on K computer. We successfully performed a RI-MP2/cc-pVTZ calculation of π-π stacked two-layer nanographene sheets $(C_{96}H_{24})_2$ (6432 atomic orbitals) on K computer. The calculation was finished in 33 minutes using 2048 node and 16384 CPU cores of K computer.

[1] Katouda, M., Nagase, S. *Int. J. Quant. Chem.*, 109:1–12, 2009.
[2] Katouda, M., Nakajima, T., Nagase, S. Proceedings of JSST 2012, 338–343, 2012.