Acceleration of divide-and-conquer method on GPU

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I. Introduction

The conventional Hartree-Fock (HF) calculations have the bottleneck at the diagonalization and construction of the Fock matrix, of which computational costs formally scale as N^3 and N^4, respectively, where N represents the size of the system under consideration. As the acceleration of diagonalization of the Fock matrix, we have implemented and assessed the divide-and-conquer (DC) self-consistent field (SCF) method. DC method is a linear-scaling scheme by dividing a total system into several subsystems originally proposed by Yang [1,2]. On the other hand, the almost 90% of computational cost is the construction of the Fock matrix. Unlike to the diagonalization, the construction has the high parallelization efficiency and the wall time could be cut down by graphical processor units (GPUs). Furthermore, the resolution-of-identity (RI) approximation [3] could reduce the construction costs. In this presentation, we will report the implementation of the DC method with GPU and show some performances.

II. Divide-and-conquer based resolution-of-identity Hartree-Fock

In the DC-HF method, we solve the Roothann-Hall equation corresponding to individual subsystem $S(\alpha)$. The local Fock matrix is constructed in the usual manner:

$$F^{\alpha}_{\mu\nu} = H^{\alpha}_{\mu\nu} + \sum_{\alpha} \sum_{\lambda\sigma\in S(\alpha)} \left[D^{a}_{\lambda\sigma} \left(\mu\nu|\lambda\sigma\right) - 1/2\, D^{a}_{\lambda\sigma} \left(\mu\lambda|\nu\sigma\right) \right]$$

$\mathbf{F}^{\alpha}$, $\mathbf{H}^{\alpha}$, and $\mathbf{D}^{\alpha}$ are the local Fock, core Hamiltonian, and density matrices. RI technique involves approximation the costly four-center two-electron integrals with the use of two-center and three-center integrals.

$$\left(\mu\nu|\lambda\sigma\right) = \sum_{P,Q} \left(\mu\nu|P\right)\left(P|Q\right)^{-1}\left(Q|\lambda\sigma\right)$$

Hereafter, indices μ, ν, λ, and σ refer to atomic orbitals (AOs), P and Q refer to auxiliary AOs.

III. Results

The present DC-RI-HF method with GPU was assessed in calculations of a oligoglycine $(gly)_{10}$. In the DC calculations, one amino acid was adopted as a central region and several adjacent left-and-right 2 units were treated as the corresponding buffer region. Table 1 shows the wall time [min] of each SCF parts (the construction of Fock matrix and diagonalization of SCF equation) by the direct-SCF and RI-SCF. The utilization of GPU reduced drastically the construction time. By the hybrid of GPU and the RI method, we achieved 10.6x speeding up of the construction time. On the other hand, the DC method could speed up the diagonalization time, which it is difficult to parallel. In the presentation, we will report the DC-based correlation methods: DC-MP2 and CCSD.

Table 1. The wall time [min] of construction of Fock matrix and diagonalization of SCF equation by direct-SCF and RI-SCF on CPU and GPU.

	Construction	Diagonalization	Total time	Speed up
Direct-HF(CPU)	124.2	3.8	128.5	-
Direct-HF(GPU)	26.7	3.8	30.7	4.2x
RI-HF(GPU)	11.7	3.8	15.9	8.1x
DC-RI-HF(GPU)	11.7	2.5	14.7	8.8x

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