Peformance Evaluation of Multiple-inputs Parallel Hatree-Fock Calculation

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Introduction

Currently, there are many research projects developing exascale supercomputer systems. To build up exascale computer systems, it is imperative to use many-core processors, which will have 16 or larger-ways SIMD functional units from requirements of high performance and low power consumption[1]. However, conventional Restricted Hatree-Fock (RHF) molecular orbital calculations have quite low SIMD operation level parallelization for the two-electron Fock-matrix (G-matrix) calculation, which is the bottleneck of RHF program. There are many GPGPU studies[2] for accelerations of Hartree-Fock or density-functional theory calculations. However, there are no analyses of SIMD operation efficiency and mainly thread level parallelizations have been utilized for accelerations. In this research, we propose a RHF calculation method which calculates multiple-inputs of different molecular structures in parallel, and those calculations are applied for SIMD parallel operations. We evaluate maximum performances for our method with test inputs whose structure data are same.

Multiple-inputs RHF calculation

Generally, for improving SIMD operation efficiency, target program has to be implemented as follows: (1) array elements of multiple-input data are aligned as continuous memory addresses for efficient vector-load and store operations, (2) data are aligned in adequate memory address boundaries, and (3) array notations are utilized for the SIMD operation regions (Intel compiler extension). According to these rules, we implemented the G-matrix calculation of multiple-input data. Except for G-matrix calculation, data were allocated at independent memory regions and original sequential codes were reused at loop body regions of multiple-input loop calculations.

Performance evaluations

We evaluated our proposed method for calculation of $(H_2O)_8$ by three types of desktop computers with Xeon 2-way X5650, 2 and 4-way E5-2650, and 8-way Phi processors. Execution times and hardware counter values were measured by PAPI library for the MPI parallel G-matrix calculations, and SIMD execution efficiencies are evaluated by following speed-up ratio.

$$Speedup\ Ratio = T_{exec}(1\,input) * N \,/\, T_{exec}(N\,inputs),$$

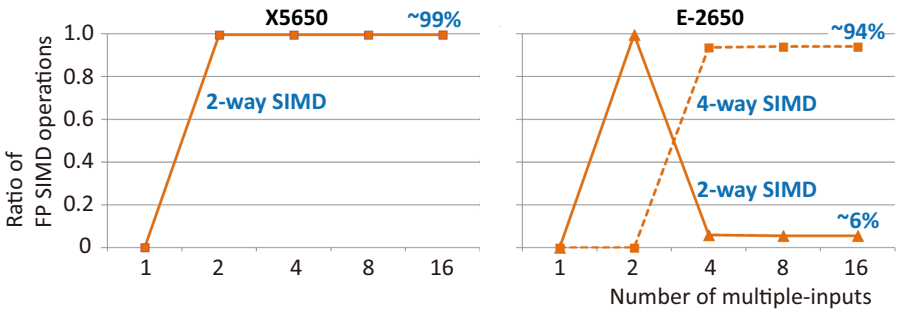

Fig. 1. Ratios of numbers of floating-point SIMD operations

Table 1. Results of effective GFLOP/s, execution efficiency, and speed-up ratios

Processor	Effective GFLOP/s[1]		Exec.efficiency (%)[2]		Speed-up
	1 input	16 inputs	1 input	16 inputs	Ratio
X5650 (2-way)	4.42	8.08	6.90	12.61	1.82
E5-2650 (2,4-way)	3.88	7.67	4.04	7.99	1.97
Phi (8-way)	1.23	7.16	0.23	1.35	5.84

1) Flop-counts are measured from one-input executions using X5650
2) Peak performance are 64.08, 128.00, and 1047.36 GFLOP/s, respectively

where $T_{exec}(N\,inputs)$ represents execution time of N inputs calculation.

Figure 1 shows the ratios of double precision floating-point (FP) SIMD operations. As number of inputs increases from 1 to 16, ratios of FP SIMD operations increase from 0% to 99.7% and from 0% to 94.0% for 2-way FP SIMD X5650 and 4-way SIMD E5-2650, respectively. Corresponding to these high ratios of 16 multiple-inputs, as shown in Table 1, we achieved 12.61%, 7.99%, 1.35% execution efficiencies and 1.82, 1.97, and 5.84 times speed-ups for Intel Xeon X5650, E5-2650, and Phi processor computers, respectively. It is expected that multiple-input parallel calculation will improve the SIMD operation efficiency for practical quantum chemistry calculations of almost same molecular geometries.

References

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