Numerical Computation

Implementation of Parallel 3-D Real FFT with 2-D Decomposition on Intel Xeon Phi Clusters

Background

The fast Fourier transform (FFT) is an algorithm which is currently widely used in science and engineering. A typical decomposition for performing a parallel 3-D FFT is slabwise. This becomes an issue with very large MPI process counts for a massively parallel cluster of many-core processors.

Overview

We proposed an implementation of a parallel 3-D real FFT with 2-D decomposition on Intel Xeon Phi clusters. The proposed implementation of the parallel 3-D real FFT is based on the conjugate symmetry property of the discrete Fourier transform (DFT) and the row-column FFT algorithm. We vectorized FFT kernels using the Intel Advanced Vector Extensions 512 (intel AVX-512) instructions.

Performance

To evaluate the implemented 3-D real FFT with 2-D decomposition, referred to as FFTE 7.0 (2-D decomposition), we compared its performance with that of the FFTE 7.0 (1-D decomposition), the FFTW 3.3.8 and the P3DFFT 2.7.7. The performance results demonstrate that the proposed implementation of parallel 3-D real FFT with 2-D decomposition effectively improves performance by reducing the communication time for larger numbers of MPI processes on Intel Xeon Phi clusters.

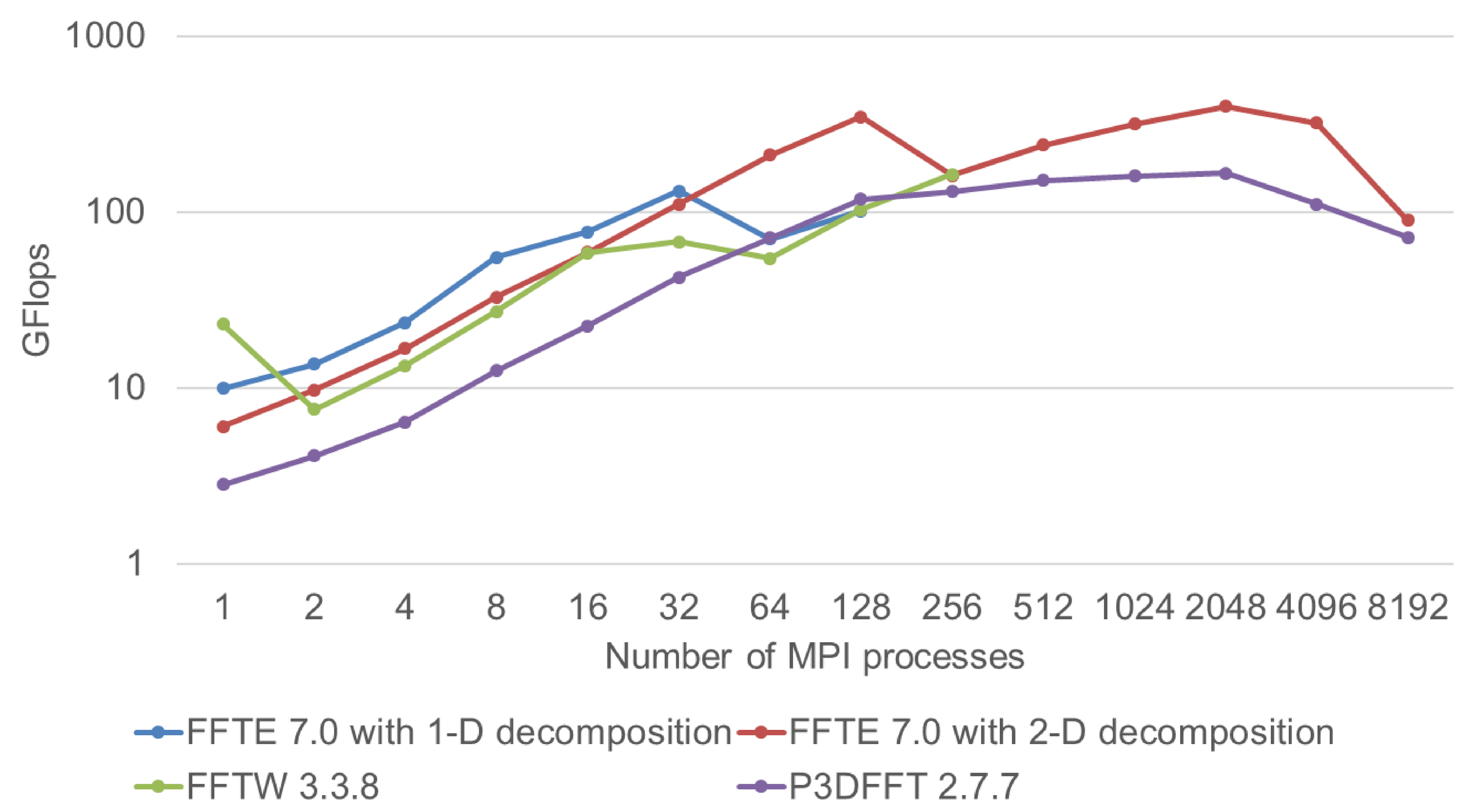

Fig. 1: Performance of Parallel 3-D Real FFTs (*N* = 256 × 512 × 512)

Development of the high accurate Block Krylov solver

Linear systems with multiple right-hand sides appear in many scientific applications such as the computation of physical quantity in lattice Quantum Chromodynamics (QCD), inner problems of eigensolvers for sparse matrix, and so on. As numerical methods for solving these linear systems, it is known that Block Krylov subspace methods are efficient methods in terms of the number of iterations and the computation time. However, the accuracy of the obtained solution may often deteriorate due to the error occurs in the computation of matrix-matrix multiplications. To improve the accuracy of the obtained solution, we have developed the new Block Krylov subspace method named Block GWBiCGSTAB method [1]. The Block GWBiCGSTAB method is based on the group-wise updating technique. By using this technique, the matrix-matrix multiplications that cause accuracy degradation can be avoided. As shown in Fig. 1, the accuracy of the obtained solution generated by the Block GWBiCGSTAB method is higher than that by other methods.

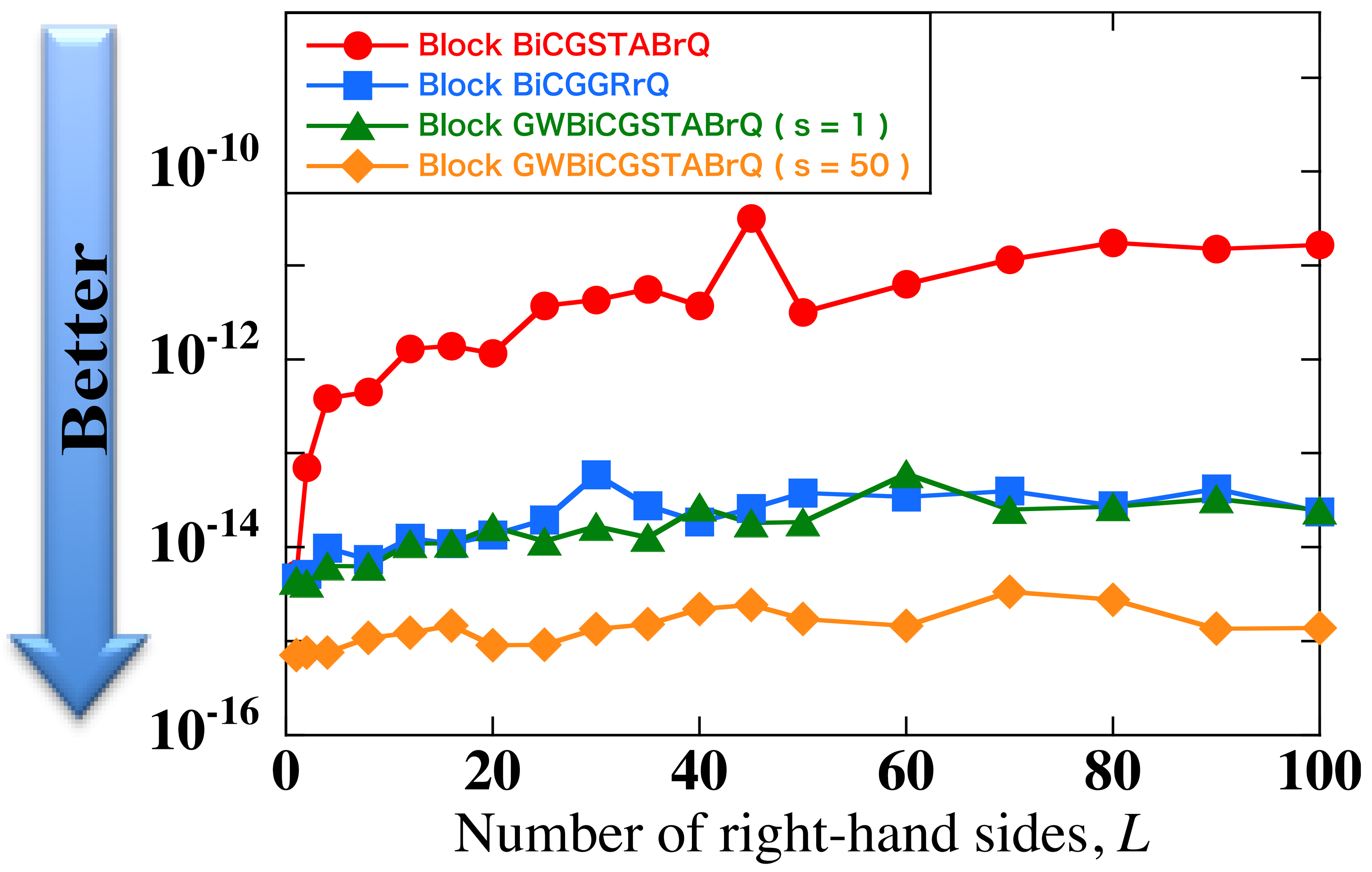

Fig. 2: True relative residual norm as a function of the number L of right-hand sides. The test problem is the linear system derived from the lattice QCD calculation. Problem size: 1,572,864.

[1] Hiroto Tadano and Ryosei Kuramoto, Accuracy improvement of the Block BiCGSTAB method for linear systems with multiple right-hands sides by group-wise updating technique, J. Adv. Simulat. Sci. Eng., Vol. 6, No. 1, pp. 100—117, 2019.