Implementation of Parallel 3-D Real FFT with 2-D Decomposition on Manycore Clusters

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Outline

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Background (1/2)

- The fast Fourier transform (FFT) is an algorithm widely used today in science and engineering.
- Parallel 3-D FFT algorithms on distributed-memory parallel computers have been well studied.
- November 2024 TOP500 Supercomputing Sites
  - El Capitan: 1,742.00 PFlops (11,039,616 Cores)
  - Frontier: 1,353.00 PFlops (9,066,176 Cores)
  - Aurora: 1,012.00 PFlops (9,264,128 Cores)
- Recently, the number of cores keeps increasing.

Background (2/2)

- A typical decomposition for performing a parallel 3-D FFT is slabwise.
  - A 3-D array $x(N_1, N_2, N_3)$ is distributed along the third dimension N_3.
  - N_3 must be greater than or equal to the number of MPI processes.
- This becomes an issue with very large MPI process counts for a massively parallel cluster of many-core processors.

Related Works

- P3DFFT [Pekurovsky 2012]
  - 3-D real-to-complex/complex-to-real FFT with 2-D decomposition
- 2DECOMP&FFT [Li and Laizet 2010]
  - 3-D complex-to-complex and real-to-complex/complex-to-real FFT with 2-D decomposition
- PFFT [Pippig 2013]
  - 3-D complex-to-complex and real-to-complex/complex-to-real FFT with 2-D decomposition

Objectives

- Implementation and evaluation of highly scalable 3-D real FFT with 2-D decomposition on manycore clusters.
- Reduce the communication time for larger numbers of MPI processes.
- A comparison between 1-D and 2-D decomposition for 3-D real FFT.

3-D DFT

- 3-D discrete Fourier transform (DFT) is given by

$$y(k_1, k_2, k_3) = \sum_{j_1=0}^{n_1-1} \sum_{j_2=0}^{n_2-1} \sum_{j_3=0}^{n_3-1} x(j_1, j_2, j_3)\, \omega_{n_3}^{j_3 k_3} \omega_{n_2}^{j_2 k_2} \omega_{n_1}^{j_1 k_1},$$

$$0 \le k_r \le n_r - 1,\ \omega_{n_r} = e^{-2\pi i/n_r}, 1 \le r \le 3$$

Real DFT

- When the input data of the DFT are real, two n-point real DFTs can be computed using an n-point complex DFT.
- Let

$$x_j = a_j + i b_j, \qquad 0 \le j \le n-1,$$

where $a_{0,} a_1, \cdots, a_{n-1}$ and $b_{0,} b_1, \cdots, b_{n-1}$ are n-point real input data.

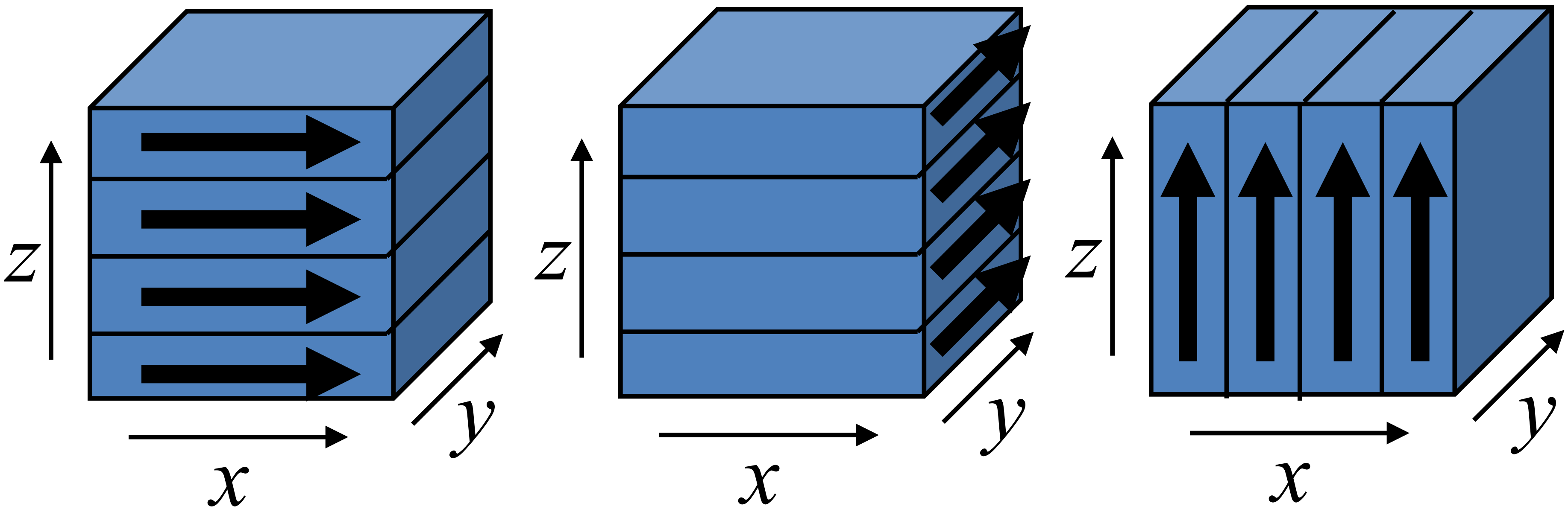
- We obtain two n-point real DFTs as follows:

$$\begin{aligned} X_k &= A_k + i B_k \\ \overline{X_{n-k}} &= A_k - i B_k \\ A_k &= \frac{1}{2}\left(X_k + \overline{X_{n-k}}\right) \\ B_k &= -\frac{i}{2}\left(X_k - \overline{X_{n-k}}\right), \qquad 0 \le k \le n/2, \end{aligned}$$

where $A_{0,} A_1, \cdots, A_{n/2}$ and $B_{0,} B_1, \cdots, B_{n/2}$ are $(n/2+1)$-point complex output data.

1-D Decomposition along the z-axis

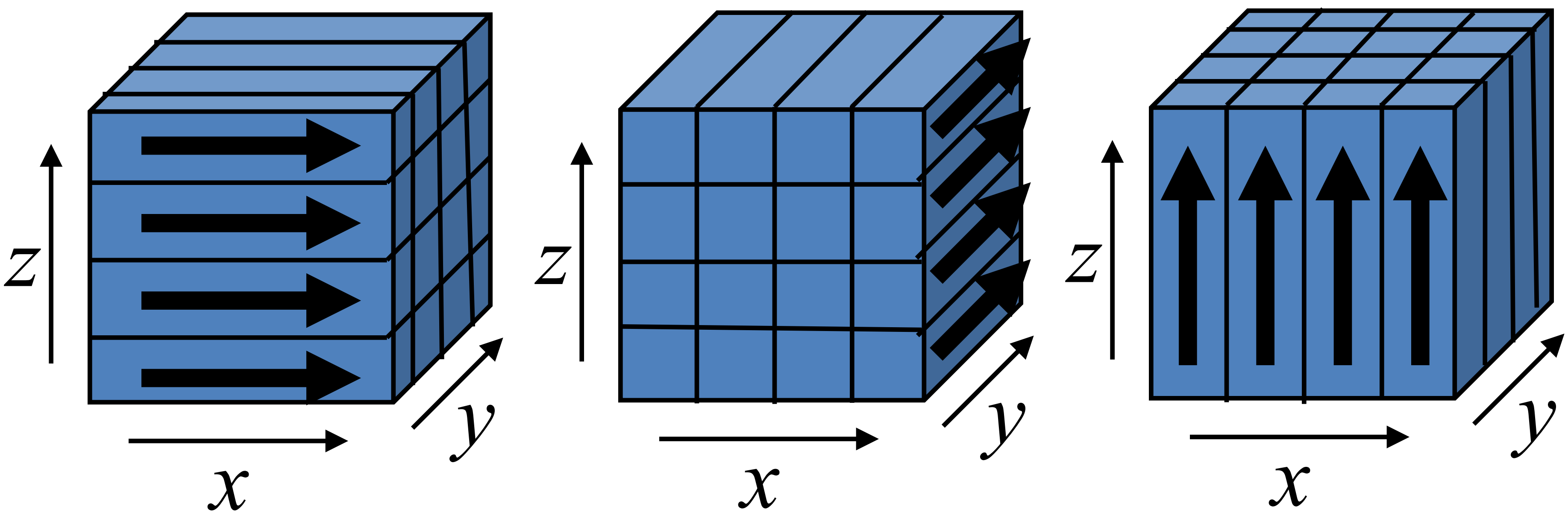
1. FFTs in x-axis　2. FFTs in y-axis　3. FFTs in z-axis



With a slab decomposition

2-D Decomposition along the y- and z-axes

1. FFTs in x-axis 2. FFTs in y-axis 3. FFTs in z-axis



With a pencil decomposition

Communication Time of 1-D Decomposition

- Let us assume for $N = N_1 \times N_2 \times N_3$-point real FFT:
  - Latency of communication: L (sec)
  - Bandwidth: W (byte/sec)
  - The number of MPI processes: $P \times Q$
- One all-to-allv communication among $P \times Q$ MPI processes
- Communication time of 1-D decomposition

$$T_{1\mathrm{dim}} \approx (PQ-1)\left(L + \frac{8N}{(PQ)^2 \cdot W}\right) \approx PQ \cdot L + \frac{8N}{PQ \cdot W} \ (\mathrm{sec})$$

Communication Time of 2-D Decomposition

- Q simultaneous all-to-allv communications among P MPI processes in the y-axis.
- P simultaneous all-to-all communications among Q MPI processes in the z-axis.
- Communication time of 2-D decomposition

$$T_{2\mathrm{dim}} \approx (P-1)\left(L+\frac{8N}{P^2Q\cdot W}\right)+(Q-1)\left(L+\frac{8N}{PQ^2\cdot W}\right)$$

$$\approx (P+Q)\cdot L+\frac{16N}{PQ\cdot W}\ (\mathrm{sec})$$

Comparing Communication Time

- Communication time of 1-D decomposition

$$T_{1\mathrm{dim}} \approx PQ \cdot L + \frac{8N}{PQ \cdot W}\ (\mathrm{sec})$$

- Communication time of 2-D decomposition

$$T_{2\mathrm{dim}} \approx (P + Q) \cdot L + \frac{16N}{PQ \cdot W}\ (\mathrm{sec})$$

- By comparing two equations, the communication time of the 2-D decomposition is less than that of the 1-D decomposition for larger number of MPI processes $P \times Q$ and latency L.

In-Cache FFT Algorithm and Vectorization

- For in-cache FFT, we used radix-2, 3, 4, 5, and 8 FFT algorithms based on the mixed-radix FFT algorithms [Temperton 83].
- Automatic vectorization was used to access the Intel AVX-512 instructions on the Xeon Phi processor.
- Although higher radix FFTs require more floating-point registers to hold intermediate results, the Xeon Phi processor has 32 ZMM 512-bit registers.

Optimization of Parallel 3-D Real FFT on Xeon Phi Processor

```
      COMPLEX*16 A(NNYY*NNZZ,*),B(NX/2+1,*),C(NY,*)
!$OMP PARALLEL DO COLLAPSE(2) PRIVATE(I,J,JJ)
      DO II=1,NX/2+1,NB
        DO JJ=1,NNYY*NNZZ,NB
          DO I=II,MIN(II+NB-1,NX/2+1)
            DO J=JJ,MIN(JJ+NB-1,NNYY*NNZZ)
              A(J,I)=B(I,J)
            END DO
          END DO
        END DO
      END DO
      …
!$OMP PARALLEL DO
      DO K=1,NNZZ*(NNXY/2+1)
        CALL IN_CACHE_FFT(C(1,K),NY)
      END DO
      …
```

To expand the outermost loop, the double-nested loop can be collapsed into a single-nested loop.

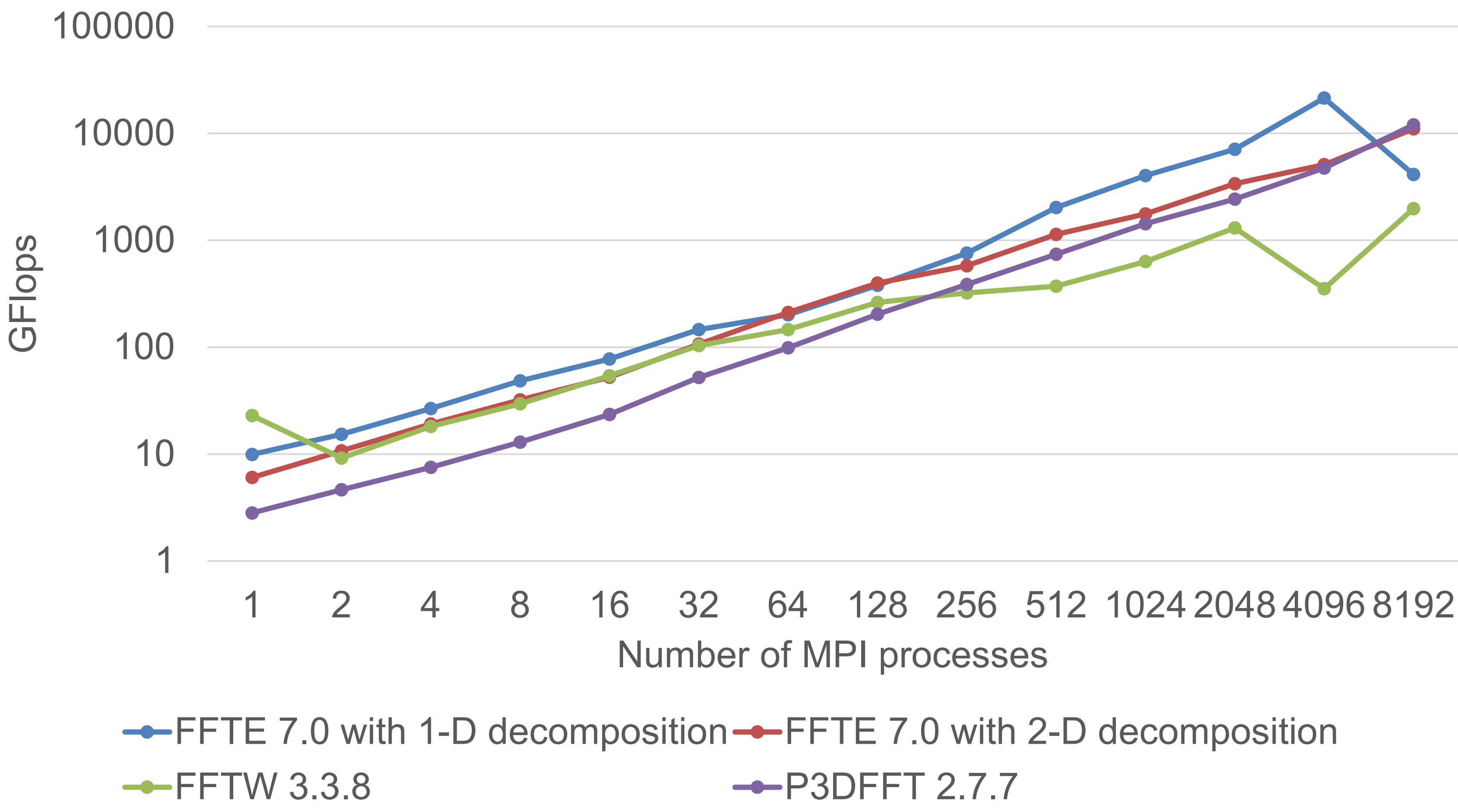
Performance Results

- To evaluate the parallel 3-D real FFT with 2-D decomposition, we compared
  - The implemented parallel 3-D real FFT, referred to as FFTE (version 7.0)
  - FFTW (version 3.3.8)
  - P3DFFT (version 2.7.7)
- Weak scaling ($N = 256 \times 512 \times 512 \times$ MPI processes) and strong scaling ($N = 256 \times 512 \times 512$) were measured.

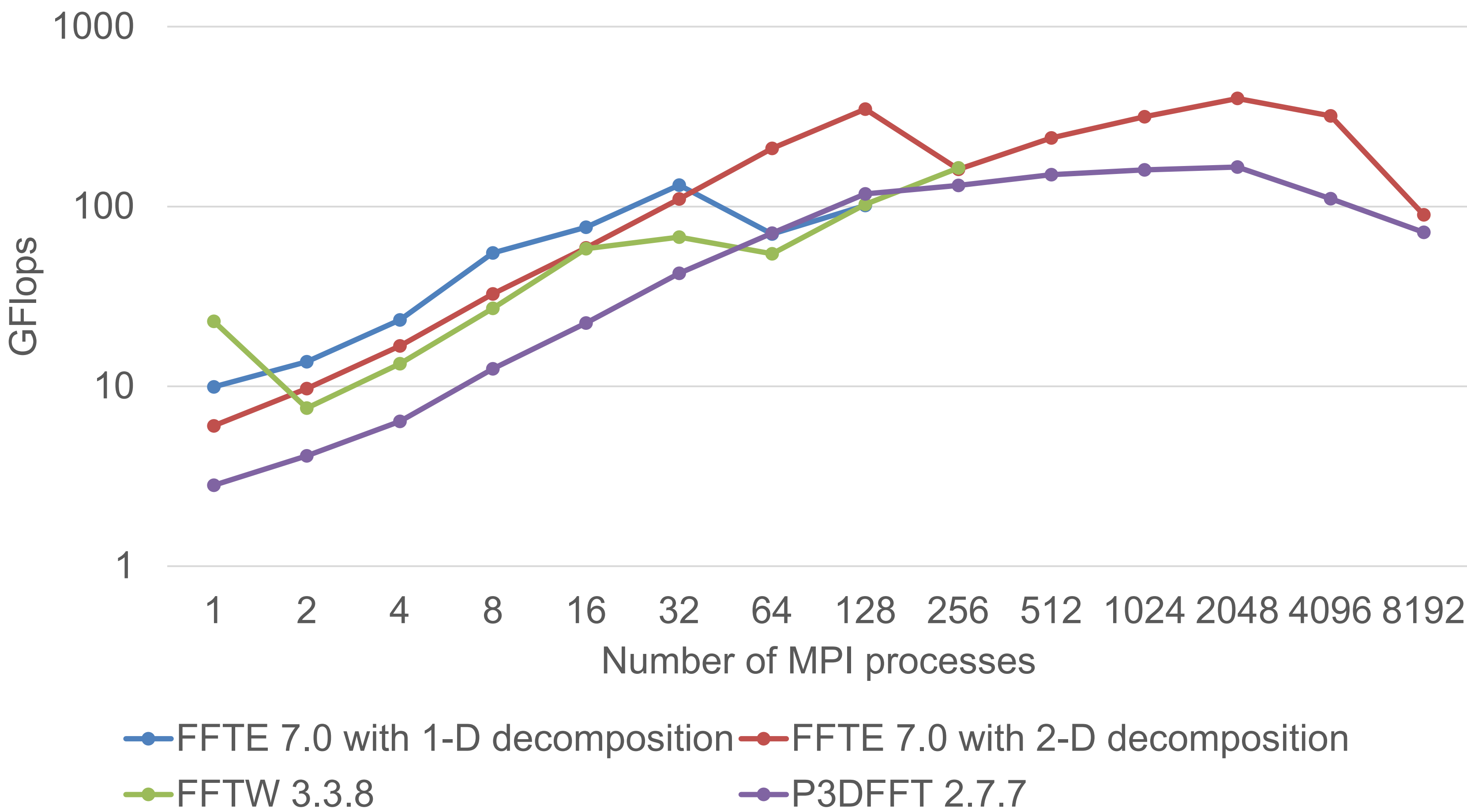
Evaluation Environment

- Oakforest-PACS at Joint Center for Advanced HPC (JCAHPC).
  - 8208 nodes, Peak 25.008 PFlops
  - CPU: Intel Xeon Phi 7250 (68 cores, Knights Landing 1.4 GHz)
  - Interconnect: Intel Omni-Path Architecture
  - Compiler: Intel Fortran compiler 18.0.1.163 (for FFTE and P3DFFT)
Intel C compiler 18.0.1.163 (for FFTW and P3DFFT)
  - Compiler option: “-O3 -xMIC-AVX512 -qopenmp”
  - MPI library: Intel MPI 2018.1.163
  - flat/quadrant, MCDRAM only, KMP_AFFINITY=balanced
  - Each MPI process has 16 cores and 64 threads,
i.e. 4 MPI processes per node.

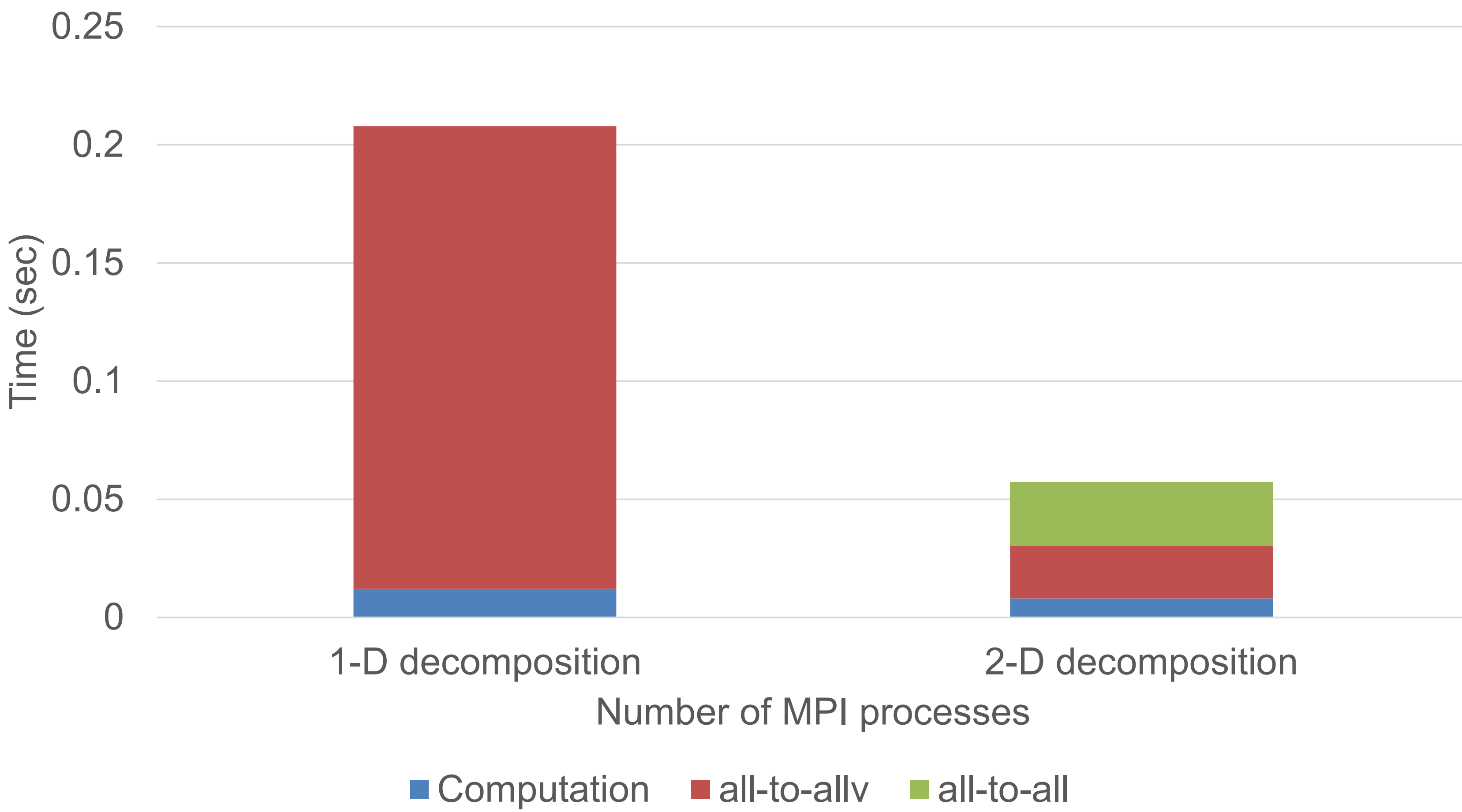
Performance of Parallel 3-D Real FFTs ($N = 256 \times 512 \times 512 \times$ MPI processes)



Performance of Parallel 3-D Real FFTs ($N = 256 \times 512 \times 512$)



Breakdown of Execution Time in FFTE 7.0 ($N = 1024^3$, 512 MPI processes)



Conclusion

- We proposed an implementation of parallel 3-D real FFT with 2-D decomposition on manycore clusters.
- The proposed parallel 3-D real FFT algorithm is based on the conjugate symmetry property for the DFT and the multicolumn FFT algorithm.
- We showed that a 2-D decomposition effectively improves performance by reducing the communication time for larger numbers of MPI processes.
- The performance results demonstrate that the proposed implementation of a parallel 3-D real FFT with 2-D decomposition is efficient for improving the performance on manycore clusters.