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Computation-Communication Overlap and Parameter Auto-Tuning for Scalable Parallel 3-D FFT

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Abstract

Parallel 3-D FFT is widely used in scientific applications, therefore it is important to achieve high performance on large-scale systems with many thousands of computing cores. This paper describes a new method for scalable high-performance parallel 3-D FFT. We use a 2-D decomposition of 3-D arrays to increase scaling to a large number of cores. In order to achieve high performance, we use non-blocking MPI all-to-all operations and exploit computation-communication overlap. We also auto-tune our 3-D FFT code efficiently in a large parameter space and cope with the complex trade-off in optimizing our code in various system environments. According to experimental results from two systems, our method computes parallel 3-D FFT significantly faster than three existing libraries, and scales well to at least 32,768 compute cores.

Keywords: 3-D FFT; MPI; Non-Blocking Collective; Computation-Communication Overlap; Auto-Tuning

1. Introduction

It is important to achieve high performance of the Fast Fourier Transform (FFT) as FFT is widely used in many fields of science and engineering. For example, researchers have recently used three-dimensional FFT (3-D FFT) to run astrophysical N -body simulations [1] and turbulent flow simulations [2] on high-performance computing systems. Computing 3-D FFT requires a large number of floating point and memory access operations. So we need a parallel algorithm that can be run on a large-scale system. However, parallel 3-D FFT requires expensive all-to-all communication. Each parallel computing process exchanges a 3-D array with all the other processes. We believe that it would be beneficial to overlap expensive computation and communication in achieving high performance of parallel 3-D FFT.

In this paper, we present a new method for parallel 3-D FFT that can increase scaling to a large number of computing cores in a distributed-memory parallel system, and exploits computation-communication overlap.¹ We design a scalable method by following the 2-D domain decomposition technique [4, 5, 6, 7, 8] that decomposes a 3-D array along two dimensions. Accordingly, we can use more computing cores than the approaches presented in [9, 10, 11] that use the 1-D domain decomposition and only decompose an array along one dimension. We exploit the overlap of computation and communication by

using the non-blocking `MPI_Ialltoall` operation that is described in the MPI-3.0 standard [12]. As the MPI library is widely used in the parallel computing community, it is important to design a parallel 3-D FFT code based on MPI and achieve portability. We use collective communication instead of point-to-point communication due to its better performance and simplicity. The MPI collectives are optimized for complex communication patterns among parallel processes, and we can write a simple code based on collective operations.

Our work is the first to effectively apply non-blocking MPI collectives to the 2-D decomposition technique for parallel 3-D FFT. Popular FFT libraries [4, 5, 9] do not exploit non-blocking communication. Although the work by Nishtala et al. [8] overlaps computation and communication, it is written in UPC and based on point-to-point communication. Hoeffler et al.'s work [10] and our previous work [11] use `MPI_Ialltoall`, but their scalability is limited as they use a 1-D domain decomposition.

Our strategy for computation-communication overlap is to have each process divide an array into multiple small blocks, and repeat computation and non-blocking communication on the divided blocks. In this way, we have opportunities to overlap computation on one block with communication on other blocks, and eventually increase the overall performance. We also increase scaling by applying our overlap strategy to each of the two communication phases in the 2-D decomposition technique for parallel 3-D FFT.

To optimize the overall performance of our method, we identify and resolve the following requirements. First, *all possible computation steps should be used for the overlap.*

¹Note that this paper is an extended version of our previous paper [3], so the two papers share several figures and texts.

Parallel 3-D FFT involves three steps of pre-computation, communication, and post-computation. Simpler approaches given in [8, 10, 13] can only overlap pre-computation on one data block with communication on other blocks, then perform post-computation on the entire blocks. Instead, we have both pre-computation and post-computation overlapped with communication. Second, *computation should be balanced between the two communication phases*. The 2-D decomposition method involves two phases of all-to-all communication, and there exist three local computation steps before and after each phase. When the communication time is different between two phases, we divide the computation in the middle into two. We then assign a longer computation to the phase with the longer communication. In this way, we increase the opportunity to overlap the computation in the middle with communication. Third, *code should be portable*. One way to ensure fully asynchronous communication for non-blocking MPI collectives is to offload communication processing to special hardware. Instead, we choose another option for asynchronous communication, which calls `MPI_Test` periodically, due to its greater portability. Last, *we should automatically handle the complex trade-off regarding our optimization techniques*. We parameterize our parallel 3-D FFT code and auto-tune the parameters. For example, a data block size for communication and a `MPI_Test` call frequency are set by tunable parameters. Since the parameter space is very large (more than trillions of possible configurations), hand-tuning is not feasible. We utilize the publicly available Active Harmony auto-tuning library [14] and find a good parameter configuration efficiently. We also introduce several techniques to tune our FFT code fast and effectively.

We conducted experiments on two systems at NERSC using up to 32,768 compute cores. Our code performs parallel 3-D FFT faster than three other approaches. Specifically, we achieve a speedup by up to $1.83\times$ over the FFTW library [9], $2.57\times$ over the 2DECOMP&FFT library [5], and $1.95\times$ over the UPC-based code [8].

The rest of the paper is organized as follows. We first describe background information in Section 2. Sections 3 and 4 present how we design and auto-tune our parallel 3-D FFT code. We relate our evaluation and results in Section 5. Section 6 provides the related work. Finally, we conclude and discuss future work in Section 7.

2. Background

This section first reviews FFT computation and describes several basic assumptions underlying our design. We then introduce a general method for parallel 3-D FFT without any computation-communication overlap.

2.1. Fast Fourier Transform

With an input array X of N complex numbers, a one-dimensional FFT produces an output array Y of N complex numbers. When $\omega_N = e^{-\frac{2\pi}{N}i}$, $Y[k]$ is defined for

Figure 1: 2-D Domain Decomposition for Parallel 3-D FFT: An input 3-D array is divided along x and y dimensions. There are two phases of blocking all-to-all communication on sub-groups of processes.

$k = 0, 1, \dots, N - 1$ as $Y[k] = \sum_{j=0}^{N-1} X[j] \omega_N^{jk}$. The d -dimensional FFT can be computed simply as the composition of a sequence of d sets of 1-D FFTs along each dimension. For example, 3-D FFT for N^3 complex numbers can be computed by three sets of N^2 1-D FFTs along each dimension.

We make the following assumptions in this paper. First, we focus on the *forward* transform that transforms X into Y . Our approach can be easily applied to transform Y backward into X . Second, we only describe the *complex-to-complex* transform that takes an input array of complex numbers and produces an output array of complex numbers. We have also implemented the real-to-complex transform by applying our computation-communication overlap methods, but omit the details of this implementation due to space limitations. Last, we focus on the *in-place* transform and want the output to overwrite the input array. Our approach can be applied directly for the out-of-place transform where the output is written to a separate array.

2.2. 2-D Domain Decomposition for Parallel 3-D FFT

Our design for a parallel 3-D FFT basically follows the 2-D domain decomposition method. The overall procedure of the 2-D domain decomposition method consists of several steps as shown in Figure 1. We parallelize 3-D FFT with p processes, and Figure 1 shows an example of $p = 4$. An input 3-D array is divided equally into p_1 sub-arrays along the x dimension and p_2 sub-arrays along the y dimension. $p_1 = 2$ and $p_2 = 2$ in Figure 1, and process numbers are marked on each sub-array. Then each process executes the following steps on each sub-array:

1. **FFTz**: Compute 1-D FFTs along the z dimension. (Assume that elements on the z dimension are adjacent in memory.)
2. **Pack1**: Pack the 3-D sub-array data into a buffer in preparation for all-to-all communication.
3. **A2A1**: Perform blocking all-to-all communication for each group of p_2 processes.
4. **Unpack1**: Unpack the received data into the 3-D sub-array with the new memory layout such that elements on the y dimension are adjacent in memory.
5. **FFTy**: Compute 1-D FFTs along the y dimension.
6. **Pack2**: Pack the 3-D sub-array data into a buffer in preparation for all-to-all communication.

Figure 2: Parallel 3-D FFT with Computation-Communication Overlap: A sub-array is divided again into communication tiles. We repeat computation and non-blocking communication on the communication tiles.

7. **A2A2**: Perform blocking all-to-all communication for each group of p_1 processes.
8. **Unpack2**: Unpack the received data into the 3-D sub-array with the new memory layout such that elements on the x dimension are adjacent in memory.
9. **FFTx**: Compute 1-D FFTs along the x dimension.

We divide the 2-D decomposition procedure into two *communication phases*: **Phase1** includes steps from FFTz through FFTy, and **Phase2** includes the rest of the procedure.

An alternative way to compute a parallel 3-D FFT is to use the *1-D domain decomposition* that only decomposes an array along one dimension rather than two. The 2-D domain decomposition method is more scalable than 1-D decomposition since we can use more computing processes. The 2-D decomposition requires two phases of all-to-all communication, which involves more complex communication pattern than the 1-D decomposition. However, the 2-D decomposition performs communication on a small sub-group of processes while the 1-D decomposition uses a whole set of processes for all-to-all communication. Thus, when both methods can be used, the system environment determines which method is faster. The 1-D decomposition can be considered as two special cases of 2-D decomposition. One case is $p_1 = 1$, where a 3-D array is only decomposed along the y dimension. The other case is $p_1 = p$, where a 3-D array is only decomposed along the x dimension. Note that our approach supports 1-D decomposition through auto-tuning. To achieve high performance parallel 3-D FFT, we tune the value of p_1 and automatically choose between a 1-D decomposition and a 2-D decomposition.

3. Parallel 3-D FFT

This section describes the design of our new parallel 3-D FFT algorithm. We will show how we can improve the 2-D decomposition method by using the non-blocking MPI all-to-all operation. We will also define 24 tunable parameters that we use to optimize the performance of our code.

3.1. Overall Algorithm

Figure 2 shows the overall procedure of our parallel 3-D FFT. Assume that an entire input 3-D array has N_x ,

N_y , and N_z elements (complex numbers) on the x , y , and z dimensions, respectively. Each of $p = p_1 \times p_2$ processes is assigned a sub-array of $\frac{N_x}{p_1} \times \frac{N_y}{p_2} \times N_z$ elements. The 3-D FFT performance can depend on how p is decomposed into $p_1 \times p_2$. So we introduce a decomposition parameter D to represent the value of p_1 . Section 4 will discuss the method to auto-tune D and other parameters of our 3-D FFT code. The memory layout for the sub-array starts with x - y - z in the row-major order. The elements on the z dimension are adjacent in memory.

We divide the FFTy step in Figure 1 into two steps of **FFTy1** and **FFTy2** as shown in Figure 2. The computation amount of each divided step is determined by a parameter R_y that is an integer number ranging from 0 through 10. FFTy1 performs 1-D FFT computation on $\frac{R_y}{10}$ of the total 1-D arrays along the y dimension during Phase1, and we finish the rest of 1-D FFT at the FFTy2 step in Phase2. By adjusting R_y properly, we can balance the FFTy computation between two communication phases and have a good chance to optimize the overlap. For example, suppose that communication in each phase takes time longer than one 1-D FFT step but shorter than two. If we perform the whole FFTy step in Phase1 like in Figure 1, a part of computation cannot be overlapped with communication. In this case, we divide the FFTy step and distribute it over two phases, so that all 1-D FFT computation can be overlapped with communication.

To fulfill the overlap during Phase1, we divide a 3-D sub-array into multiple small blocks along the x dimension as shown in Figure 2. We call each divided block a *communication tile*. We define a tile size parameter T_1 to handle the trade-off between the overlap efficacy and the messaging efficiency. With small T_1 , we can overlap many computations with communication but there would be a large overhead of exchanging many small-sized messages. If T_1 gets bigger, there will be less overlap but higher efficiency for communication. Thus we should find a good value of T_1 to achieve high performance. Each tile contains T_1 elements on the x dimension. So the number of elements in each communication tile is equal to $T_1 \times \frac{N_y}{p_2} \times N_z$. We also define a window size parameter W_1 to specify the degree of communication parallelism. It is also important to adjust W_1 properly to utilize as many concurrent communication connections as possible.

Algorithm 1 describes a pseudocode for each process. Each process repeats the FFTz, Pack1, A2A1, Unpack1, and FFTy1 steps for each communication tile. Unlike the original 2-D decomposition method, Algorithm 1 uses the non-blocking MPI all-to-all operation (`MPI_Ialltoall` and `MPI_Wait`) for the A2A1 step. Thus we can overlap computation (FFTz, Pack1, Unpack1, and FFTy1) on one communication tile with communication (A2A1) for other tiles. After the Unpack1 step, the data in each communication tile are rearranged in memory to the x - z - y order, so that we can execute the FFTy1 step on 1-D arrays along the y dimension. To achieve high performance for the 1-D FFT computation steps, we utilize the highly optimized

Algorithm 1: Parallel 3-D FFT on Each Process

```

1  1 Divide data into  $k_1 = \lceil \frac{N_x}{p_1} / T_1 \rceil$  tiles on the  $x$  dimension
2
3  2 for  $i \leftarrow 0$  to  $k_1 + W_1 - 1$  do
4
5      3 if  $i < k_1$  then FFTz & Pack1 on tile  $i$ 
6
7      4 if  $i \geq W_1$  then MPI_Wait on tile  $(i - W_1)$ 
8
9      5 if  $i < k_1$  then MPI_Ialltoall on tile  $i$ 
10
11     6 if  $i \geq W_1$  then Unpack1 & FFTy1 on tile  $(i - W_1)$ 
12
13  7 Transpose: Change the memory layout  $x$ - $z$ - $y \rightarrow z$ - $x$ - $y$ 
14
15  8 Divide data into  $k_2 = \lceil \frac{N_z}{p_2} / T_2 \rceil$  tiles on the  $z$  dimension
16
17  9 for  $i \leftarrow 0$  to  $k_2 + W_2 - 1$  do
18
19     10 if  $i < k_2$  then FFTy2 & Pack2 on tile  $i$ 
20
21     11 if  $i \geq W_2$  then MPI_Wait on tile  $(i - W_2)$ 
22
23     12 if  $i < k_2$  then MPI_Ialltoall on tile  $i$ 
24
25     13 if  $i \geq W_2$  then Unpack2 & FFTx on tile  $(i - W_2)$ 

```

code from the FFTW library [9].

There are at most W_1 tiles with active communication being executed. While the process is working on a tile for the FFTz and Pack1 steps, the all-to-all communication (A2A1) for the previous W_1 tiles takes place in the background. Also, when the process is working on a tile for Unpack1 and FFTy1, the communication for the next W_1 tiles goes on in the background. Likewise, during A2A1 on tile i , the previous W_1 tiles are computed for Unpack1 and FFTy1, and the next W_1 tiles are computed for FFTz and Pack1.

Before starting Phase2, Algorithm 1 runs the **Transpose** step and changes memory layout to the z - x - y order. We need the Transpose step because we divide data into communication tiles along the z dimension in Phase2. For the Transpose step, the FFTW *guru* interface is used to execute a high-performance routine of memory rearrangement.

Likewise, we introduce parameters of T_2 and W_2 to represent communication tiles during Phase2. Algorithm 1 repeats the FFTy2, Pack2, A2A2, Unpack2, and FFTx steps for each communication tile. Similarly to Phase1, we overlap computation (FFTy2, Pack2, Unpack2, and FFTx) on one communication tile with communication (A2A2) for other tiles in Phase2. The final memory layout is z - y - x .

3.2. Fully Asynchronous Communication

In order to achieve a computation-communication overlap, the non-blocking MPI all-to-all communication should make progress while computation takes place. Among several methods [15] for fully asynchronous communication, we choose the *manual progress* method, which is to call MPI_Test periodically during computation. MPI collection communication involves multiple point-to-point communication rounds, and calling MPI_Test lets the MPI library move on to the next round of point-to-point communication. Accordingly, our code achieves portability and does not require any hardware support or separate threads for computation-communication overlap.

Figure 3: Loop Tiling for Cache Reuse: A communication tile is divided again into sub-tiles. We can increase cache hits during local computation by reading the sub-tile information from a cache.

It is important to determine the proper frequency of MPI_Test calls. Too high frequency will incur unnecessary function call overhead, and too low frequency will limit the progress of the all-to-all communication. To cope with the trade-off, we have four tunable parameters to adjust the frequency of MPI_Test calls during Phase1. F_z defines the number of MPI_Test calls during FFTz for one communication tile. F_{p1} is the frequency parameter during the Pack1 step for one communication tile. F_{u1} is for Unpack1, and F_{y1} is for FFTy1. Likewise, we introduce F_{y2} , F_{p2} , F_{u2} , and F_x for FFTy2, Pack2, Unpack2, and FFTx in Phase2.

3.3. Loop Tiling for Cache Reuse

We optimize the FFTz and Pack1 steps by tiling the loop inside each communication tile. As shown in the left side of Figure 3, each communication tile is divided again into *sub-tiles* with P_{x1} elements on the x dimension and P_{y1} on the y dimension. So each sub-tile contains $P_{x1} \times P_{y1} \times N_z$ elements. By executing FFTz and Pack1 over each sub-tile, we can increase cache hit rate during Pack1. Similarly to FFTz and Pack1, we optimize Unpack1 and FFTy1 through loop tiling. Each communication tile is divided into sub-tiles with U_{x1} elements on the x dimension and U_{z1} on z dimension. Thus, we can increase cache hits during FFTy1 by reading the sub-tile information from a cache after Unpack1. Likewise, we utilize loop tiling in the second phase as shown in the right side of Figure 3. P_{x2} and P_{z2} are used for FFTy2 and Pack2, and U_{y2} and U_{z2} are used for Unpack2 and FFTx.

3.4. Improvement Opportunities

First, there is an opportunity to improve the performance by using MPI_Ialltoallv. If a 3-D array is uniformly decomposed among all $p = p_1 \times p_2$ parallel processes, four conditions must be satisfied: 1) $N_x \bmod p_1 = 0$, 2) $N_y \bmod p_1 = 0$, 3) $N_y \bmod p_2 = 0$, and 4) $N_z \bmod p_2 = 0$. In the case of uniform domain decomposition, we can simply use MPI_Ialltoall as every process sends and receives the same amount of data. However, when any of the four conditions is not satisfied, the array cannot be uniformly decomposed. In the case of non-uniform domain decomposition, we have two options of all-to-all communication: 1) use MPI_Ialltoallv and allow each process to send a different amount of data or 2) use MPI_Ialltoall

Table 1: 24 Auto-Tunable Parameters of Parallel 3-D FFT

D	# processes on x -dim
T_1	# elements on x -dim in a communication tile (Phase1)
W_1	max # tiles for concurrent communication (Phase1)
P_{x1}	# elements on x -dim in a sub-tile during Pack1
P_{y1}	# elements on y -dim in a sub-tile during Pack1
F_z	# <code>MPI_Test</code> calls during FFTz for one tile
F_{p1}	# <code>MPI_Test</code> calls during Pack1 for one tile
U_{x1}	# elements on x -dim in a sub-tile during Unpack1
U_{z1}	# elements on z -dim in a sub-tile during Unpack1
F_{u1}	# <code>MPI_Test</code> calls during Unpack1 for one tile
F_{y1}	# <code>MPI_Test</code> calls during FFTy1 for one tile
R_y	computation ratio of FFTy1 to total FFTy
T_2	# elements on z -dim in a communication tile (Phase2)
W_2	max # tiles for concurrent communication (Phase2)
P_{z2}	# elements on z -dim in a sub-tile during Pack2
P_{x2}	# elements on x -dim in a sub-tile during Pack2
F_{y2}	# <code>MPI_Test</code> calls during FFTy2 for one tile
F_{p2}	# <code>MPI_Test</code> calls during Pack2 for one tile
U_{z2}	# elements on z -dim in a sub-tile during Unpack2
U_{y2}	# elements on y -dim in a sub-tile during Unpack2
F_{u2}	# <code>MPI_Test</code> calls during Unpack2 for one tile
F_x	# <code>MPI_Test</code> calls during FFTx for one tile
V	switch to use <code>MPI_Ialltoallv</code> or not
S	switch to use the stride method or not

after padding messages. We introduce a parameter V to decide which option we should use for non-uniform domain decomposition. If $V = 0$, we do not use `MPI_Ialltoallv`. If $V = 1$, we use `MPI_Ialltoallv` only for A2A2. If $V = 2$, we use `MPI_Ialltoallv` only for A2A1. If $V = 3$, we use `MPI_Ialltoallv` for both A2A1 and A2A2.

The second opportunity is to use the *stride method* for 1-D FFT. FFTW allows us to perform 1-D FFT on an array with stride of general N elements. If we utilize the stride method, we do not have to rearrange a memory layout for 1-D FFT computation. We can modify each step of our algorithm to maintain the x - y - z layout. Then we have an opportunity to remove the Transpose step. We introduce a switch parameter S to decide whether to use the stride method ($S = 1$) or not.

As the last improvement technique, we remove the Transpose step when $N_x = N_y$. We modify Unpack2 to generate the y - z - x layout (as opposed to z - y - x) for the case of $N_x = N_y$. Then the source and destination data for the A2A2 step will reside in the same memory area. Thus we can avoid the cost of the Transpose step and improve the overall 3-D FFT performance. We have no parameter for the third improvement technique because we always use it for the case of $N_x = N_y$.

4. Auto-Tuning

Table 1 summarizes the 24 tunable parameters contained in our parallel 3-D FFT code. Since it is impossible to investigate all the configurations manually and exhaustively, we need an efficient way to tune the parameters

Figure 4: Auto-Tuning Procedure: The Active Harmony server decides a test parameter configuration. The Active Harmony client executes 3-D FFT with the received configuration, and reports the performance back to the server.

automatically and determine a good configuration. This section introduces an auto-tuning software framework and presents how we customize the auto-tuner for fast and effective tuning.

4.1. Active Harmony

We use a general software framework called Active Harmony (AH) [14] for auto-tuning because it provides easy-to-use APIs to auto-tune user-specified parameters. Figure 4 shows the overall procedure of how AH interacts with our parallel 3-D FFT code. The AH server searches efficiently through a large parameter space and decides a parameter configuration to be tested on the tuning target (our parallel 3-D FFT code). The AH client receives a parameter configuration from the server, executes the tuning target with the received configuration, and reports the performance back to the server. This procedure is repeated until the AH server finds the best parameter configuration.

Among several strategies provided by the AH server, we use the Nelder-Mead (NM) method [16] to search for a good parameter configuration. NM is a commonly used optimization technique in many fields of science. NM uses the concept of a *simplex*, which is a polytope of $(d+1)$ vertices in d dimensions. For example, a simplex is a triangle in two dimensions. The AH client measures the performance of 3-D FFT at each point (or parameter configuration) on a simplex. NM generates a new test point by extrapolating the performance values measured at points on the simplex. Then NM replaces one of the simplex points with the new point. For example, NM sometimes replaces the worst simplex point W with a new point R such that R is reflected from W through the centroid of the remaining d points. The search procedure finishes when all the points on a simplex are close to each other, and can be considered to be converged to a single point. Further details about NM are described in [16].

4.2. Initial Simplex

An initial simplex in NM can affect the tuning time and the quality of the tuning result because a poor initial simplex could cause the search to get stuck at local minimum points. This section describes how we determine an initial simplex, and Section 5 will demonstrate its performance with experiments. We construct an initial simplex

by choosing 25 random points within a limited area of parameter space. In other words, we choose a random value for each parameter within a limited range. D is chosen from any number by which p is divisible. T_1 and T_2 are set, so that the number of elements of each tile ranges in $[2^6, 2^{22}]$. Therefore we can avoid too small or too large size of communication messages. The message size would range from a few KB to tens of MB. W_1 and W_2 are chosen in $[0, 5]$. We determine loop tiling parameters ($P_{x1}, P_{y1}, U_{x1}, U_{z1}, P_{x2}, P_{z2}, U_{y2}$, and U_{z2}) in the way that the number of elements of each sub-tile ranges in $[2^{10}, 2^{17}]$. Thus we can utilize hardware caches with the size between a few KB and a few MB. `MPI_Ialltoall` in Phase1 requires more rounds of point-to-point communication as p_2 increases. So the `MPI_Test` call frequency parameters (F_{z1}, F_{p1}, F_{u1} , and F_{y1}) are chosen in $[\frac{1}{8} \times p_2, 32 \times p_2]$. Likewise, F_{y2}, F_{p2}, F_{u2} , and F_x are chosen in $[\frac{1}{8} \times p_1, 32 \times p_1]$. Finally, we choose R_y from $[0, 10]$, V from $[0, 3]$, and S from $[0, 1]$.

4.3. Customization

We have customized the AH client by introducing several techniques for effective and fast auto-tuning. First, we *penalize an infeasible configuration*. The possible range of parameter values can be limited by other parameters. For example, $1 \leq T_1 \leq \frac{N_x}{D}$ and $1 \leq P_{x1} \leq T_1$ must be satisfied. However, the Nelder-Mead method of AH is originally designed to work in a multi-dimensional orthotope (hyper-rectangle) parameter space.² So the AH server can generate an infeasible test configuration. We customized the AH client to report the worst performance value (infinity) immediately back to the AH server when the AH client receives an infeasible configuration. Then the AH server will suggest another configuration that might be in a feasible area in the parameter space. Accordingly, our FFT code avoids any error derived from an infeasible configuration.

Second, we *utilize the tuning history*. The AH server sometimes provides the same parameter configuration even though it has been already investigated before. This happens because our parameter values exist in the discrete integer domain. Simplex points are in the continuous real domain as NM was originally designed to optimize a continuous function. Thus the AH server generates a test parameter configuration using the closest integer point to a simplex point in a continuous domain. To save tuning time, we record the history of tested configurations, and reuse the prior performance data when the AH client receives the previously tested configuration again.

Third, we *reduce a search space* to a log scale and consider power-of-two values for testing. Thus we can avoid searching a whole set of all possible values of a parameter. The minimum and maximum values are additionally considered for testing whether the value is a power of two or

not. So, we can also take into account the boundary values in the original parameter space after reducing the search space. For example, when $N_x = 640$ and $D = 32$, T_1 can be 1, 2, 4, 8, 16, or 20. As an exception, the log-scale reduction is not applied to W_1, W_2, R_y, V , and S because there are few possible values for those parameters.

The fourth technique is called *tile extrapolation*. Our 3-D FFT algorithm repeats similar computation and communication on many tiles. So the execution time on tiles will be similar to one another. To reduce the execution time of each configuration, we execute the `for`-loops in Algorithm 1 only for the first few tiles. We then estimate the whole execution time by extrapolating the measured time. When the window size is not zero, we do not start extrapolation until the communication window is filled up. For example, if $W_1 = 2$, we start extrapolation at the third tile after the first two tiles fill up the communication window.

5. Evaluation

We first introduce our experimental platforms and three other approaches to compare with our approach. Second, we describe the results of small scale experiments. We will show how fast our 3-D FFT is compared to the others, and where the improvement comes from. Then we describe the results of large-scale experiments and show how well our approach scales as the number of cores increases. Last, we quantify the auto-tuning cost.

5.1. Platforms and Comparison Models

We use two platforms for our experiments. The first platform, which is named **Edison**, is a Cray XC30 machine at NERSC. Each node consists of two 12-core Intel Ivy Bridge processors (124,608 cores total in the machine). Each core has L1 and L2 caches, with 64KB and 256KB, respectively. A 30MB L3 cache is shared between 12 cores on a processor. We used all 24 cores per node in our experiments. The Cray Aries with Dragonfly topology is used to connect nodes. For a non-blocking all-to-all operation on Edison, we used `MPI_Ialltoall` of the Cray Message Passing Toolkit 6.2.0 that is derived from the MPICH implementation. FFTW 3.3.0.4 is used. We used the Intel C and Fortran compilers and the Cray UPC compiler with `-O3` option to compile codes. The second platform is **Hopper**, a Cray XE6 machine at NERSC. Each node contains two 12-core AMD MagnyCours 2.1GHz processors (153,216 cores total in the machine). Each core has L1 and L2 caches, with 64KB and 512KB, respectively. One 6MB L3 cache is shared between six cores on a processor. We used all 24 cores per node. Nodes are connected via a Cray Gemini Network that forms a 3-D torus. We used the Cray Message Passing Toolkit 6.0.1 and FFTW 3.3.0.4. We compiled codes using the PGI C and Fortran compilers and the Cray UPC compiler with `-fast` option.

²The developers of Active Harmony recently implemented a constraint plugin that supports a non-hyperrectangle parameter space, but it was not ready when the experiments for this paper were done.

Table 2: Parallel 3-D FFT Time (seconds) and Parameter Values Found via Auto-Tuning (Small Scale)

(a) Edison

p	N^3	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
256	768 ³	0.195	1	32	5	1	1	64	32	1	2	32	64	X	X	X	X	X	X	X	X	X	X	X	0	1
256	1024 ³	0.516	1	256	1	4	4	256	16	2	4	16	1024	X	X	X	X	X	X	X	X	X	X	X	0	1
256	1280 ³	0.979	1	8	1	2	2	32	8	1	1	32	32	X	X	X	X	X	X	X	X	X	X	X	0	1
256	1536 ³	1.909	1	128	4	8	2	256	32	1	2	128	128	X	X	X	X	X	X	X	X	X	X	X	0	1
256	1792 ³	2.898	1	128	4	1	1	256	128	1	4	32	512	X	X	X	X	X	X	X	X	X	X	X	0	1
256	2048 ³	4.749	256	X	X	X	X	X	X	X	X	X	X	X	128	2	4	8	64	32	8	1	32	128	0	0
512	768 ³	0.113	128	1	2	1	32	2	1	1	8	2	8	5	8	1	8	4	16	1	2	1	8	32	0	0
512	1024 ³	0.298	32	4	3	1	8	32	8	2	2	2	32	5	8	3	2	4	64	8	2	4	8	32	0	0
512	1280 ³	0.492	32	2	4	1	8	16	2	1	32	2	8	4	4	2	2	2	32	8	1	8	8	32	0	0
512	1536 ³	1.017	1	512	2	2	1	512	64	1	2	64	1024	X	X	X	X	X	X	X	X	X	X	X	0	1
512	1792 ³	1.665	1	256	1	1	1	512	512	2	1	512	64	X	X	X	X	X	X	X	X	X	X	X	2	1
512	2048 ³	2.277	1	256	2	1	2	256	128	2	2	64	512	X	X	X	X	X	X	X	X	X	X	X	0	0

(b) Hopper

p	N^3	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
256	768 ³	0.450	32	4	2	1	4	8	4	2	4	4	16	4	4	2	2	4	32	4	2	2	8	8	0	0
256	1024 ³	1.077	8	8	2	2	4	16	16	2	4	8	32	7	4	2	1	16	8	4	2	2	8	32	0	0
256	1280 ³	2.155	16	8	2	2	8	8	2	1	1	8	128	9	2	1	2	4	2	8	1	16	2	32	0	0
256	1536 ³	3.726	1	128	5	2	1	64	128	4	4	32	512	X	X	X	X	X	X	X	X	X	X	X	0	0
256	1792 ³	5.733	1	128	1	4	4	128	16	4	2	32	256	X	X	X	X	X	X	X	X	X	X	X	0	0
256	2048 ³	8.691	256	X	X	X	X	X	X	X	X	X	X	X	128	1	1	4	128	128	8	4	32	512	0	0
512	768 ³	0.277	32	8	2	2	16	8	4	4	2	4	8	3	8	1	1	2	32	4	4	4	8	64	0	0
512	1024 ³	0.567	32	4	2	2	8	16	8	2	16	4	8	5	2	2	2	4	16	8	1	8	4	8	0	0
512	1280 ³	1.232	64	4	2	1	8	16	8	2	8	8	16	4	16	2	2	8	64	16	2	8	16	128	0	0
512	1536 ³	2.060	32	4	2	2	2	32	4	4	8	4	16	1	4	1	2	4	64	16	2	2	4	64	0	0
512	1792 ³	3.791	32	4	2	2	4	16	8	2	4	16	32	3	4	1	2	4	16	8	4	4	4	16	0	0
512	2048 ³	5.251	128	2	1	1	8	16	8	1	8	4	16	0	64	2	2	4	512	32	1	4	128	64	0	0

We compare four different methods for parallel 3-D FFT. **FFTW** is the FFTW library [9] that uses 1-D decomposition and blocking MPI communication. We tune and optimize the parallel 3-D FFT computation of FFTW by using the `FFTW_MEASURE` option. Second is **DCMP**, which is the 2DECOMP&FFT library [5] that uses 2-D decomposition and blocking MPI collective communication.³ For fair comparison with our tuned approach, we exhaustively run all the possible process grids of $p_1 \times p_2$ and choose the option with the best performance. Third, we compare our approach with **UPCF**, which is a UPC code [8] that is based on 2-D decomposition. UPCF overlaps computation with communication through one-sided point-to-point communication operations. We downloaded the UPC implementation of the NAS Parallel Benchmark FT (UPC-FT) from the NERSC website. Then we built UPCF by extracting a core part of UPC-FT containing the 3-D FFT computation. Like DCMP, UPCF tunes $p_1 \times p_2$ exhaustively. Last is **NEW**, which is our method described in Section 3. NEW is auto-tuned by the Nelder-

³We do not use P3DFFT [4] in experiments because it does not support the complex-to-complex transform. P3DFFT is reported to show the similar performance to 2DECOMP&FFT for the real-to-complex transform. [17]

Mead strategy of Active Harmony as described in Section 4. Since DCMP, UPCF, and NEW rely on the FFTW library for 1-D FFT computation, we tune those computations with the `FFTW_MEASURE` option.

5.2. Small Scale Experiments

We first performed experiments on a relatively small number (256 and 512) of compute cores. Input sizes are 768³ to 2048³ complex numbers, which are sufficiently large so that we can run FFTW and use 1-D decomposition.

5.2.1. Parallel 3-D FFT Performance

The third column of Table 2(a) shows the 3-D FFT execution time of our NEW approach on Edison. Figure 5(a) shows the speedup of NEW over other approaches. p is the number of cores used. N is the number of elements on each dimension in a 3-D input array. For each of the four algorithms being compared, we conducted five runs of tuning on different sets of computing nodes. To cope with the execution noise, we executed five runs of 3-D FFT with each of five tuning results, then picked the best performance out of the 25 runs. Figure 5(a) shows that NEW is faster than FFTW, DCMP, and UPCF for all different

(a) Edison

(b) Hopper

Figure 5: Parallel 3-D FFT Speedup of NEW Relative to Other Algorithms on Small Scale Experiments: Our NEW method has speedup of up to $1.83\times$ over FFTW (the MPI-enabled FFTW library), $1.58\times$ over DCMP (the 2DECOMP&FFT library), and $1.32\times$ over UPCF (the UPC implementation of the NAS Parallel Benchmark FT) on Edison. NEW shows speedup of up to $1.31\times$ over FFTW, $1.26\times$ over DCMP, and $1.50\times$ over UPCF on Hopper. We used all 24 cores per node of Edison and Hopper. NEW is faster with the original setting than the cross-platform setting (CRSS), which justifies the necessity of auto-tuning on different platforms.

settings of p and N . NEW has speedup of up to $1.83\times$ over FFTW, $1.58\times$ over DCMP, and $1.32\times$ over UPCF.

To better explain the effectiveness of NEW, we break down the performance of NEW for the $p = 512$ and $N^3 = 1024^3$ configuration in Figure 9(a). **NEW-0** is a non-overlapped version of NEW where W_1 , W_2 , and all the frequency parameters are set to be zero with all the other parameters equal to NEW. Also, lines 4 and 5 (also lines 11 and 12) in Algorithm 1 are replaced with `MPI_Ialltoall` and `MPI_Wait` on tile i . In Phase1, the all-to-all communication time (the `MPI_Wait` time marked with Wait1) of NEW-0 is 0.028 seconds on Edison, and NEW reduces the Wait1 time down to zero. In Phase2, the communication time (Wait2) of NEW-0 is 0.173 seconds. The Wait2 time of NEW is reduced to only 0.048 seconds as the “overlappable” computation time (FFTy2+FFTx and Pack2+Unpack2) of NEW is 0.125 seconds. So the sum of computation time and communication time of NEW is equal to the communication time of NEW-0. The reduced communication time (Wait1 and Wait2) of NEW represents NEW nearly achieves the perfect computation-communication overlap on Edison. The overhead for the computation-communication overlap is quantified as the time for calling `MPI_Test`. NEW spends 0.029 seconds for `MPI_Test` (Test1 and Test2) on Edison. Since this overhead is much shorter than the reduced communication time (Wait1 and Wait2) of NEW (0.153 seconds), NEW could successfully improve the overall FFT performance from NEW-0.

The high degree of overlap explains why NEW is faster than the other approaches. Since FFTW and DCMP do not exploit non-blocking communication, the performance is lower than NEW as shown in Figure 5(a). UPCF over-

laps computation and communication, but it is still slower than NEW. There are three possible reasons of UPCF’s low performance. First, the UPCF design [8] misses some computation (Unpack1, Unpack2, and FFTx) to overlap with communication. Second, UPCF is not able to tune the size of communication message as there is no concept of T_1 and T_2 . Last, UPCF uses the point-to-point communication while NEW is based on the optimized collective operation. Note that Wait1 of NEW-0 is shorter than Wait2 in Figure 9(a). The reason of the short communication time of Phase1 is fast intra-node communication. We map MPI processes to a 3-D array along the y dimension first as shown in Figure 2. By default, Edison uses the SMP-style mapping between MPI processes and physical cores, so it fills up one node before going to next. Thus Phase1 involves a large amount of intra-node communication, which should be faster than inter-node communication of Phase2.

We conducted the same experiment on Hopper as what we did on Edison. Table 2(b) shows the 3-D FFT execution time on Hopper. Figure 5(b) shows the speedup of NEW over the other approaches.⁴ NEW is still the fastest on Hopper (up to $1.31\times$ FFTW, $1.26\times$ DCMP, and $1.50\times$ UPCF), but the speedup is somewhat lower than the speedup on Edison. This low speedup on Hopper comes from the non-maximized overlap. In Figure 9(a), NEW on Hopper takes around 0.070 seconds for Phase2 communication (marked with Wait2), which means a non-optimized overlap. NEW is supposed to have zero communication time as the computation time (FFTy2+FFTx and

⁴UPCF crashes at $p = 256$ and $N^3 = 2048^3$ on Hopper with an out-of-memory error. UPCF requires a large amount of memory as it only supports the out-of-place transform.

Table 3: Parallel 3-D FFT Time (seconds) and Parameter Values Found via Auto-Tuning (Large Scale)

(a) Edison (Strong Scaling)

p	N^3	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
128	1024^3	0.965	4	4	3	1	8	32	8	1	4	8	16	8	8	1	4	16	4	32	2	4	32	16	0	0
256	1024^3	0.516	1	256	1	4	4	256	16	2	4	16	1024	X	X	X	X	X	X	X	X	X	X	X	0	1
512	1024^3	0.298	32	4	3	1	8	32	8	2	2	2	32	5	8	3	2	4	64	8	2	4	8	32	0	0
1024	1024^3	0.159	64	4	2	2	32	4	2	2	2	4	8	5	16	1	4	8	32	8	4	4	8	32	0	0
2048	1024^3	0.100	256	2	2	1	16	4	4	1	32	2	64	5	16	4	4	2	32	16	8	2	4	32	0	0
4096	1024^3	0.055	256	4	0	1	4	0	0	2	4	0	0	3	16	2	8	4	64	4	2	4	8	64	0	0
8192	1024^3	0.030	512	2	0	2	8	0	0	1	8	0	0	2	32	2	8	1	32	4	4	1	8	32	0	0
16384	1024^3	0.018	256	4	0	2	16	0	0	2	4	0	0	3	8	2	2	4	16	8	4	4	2	32	0	0
32768	1024^3	0.012	256	4	0	2	4	0	0	4	4	0	0	5	8	0	4	4	0	0	4	1	0	0	0	0

(b) Hopper (Strong Scaling)

p	N^3	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
128	1024^3	1.673	128	X	X	X	X	X	X	X	X	X	X	X	64	5	2	8	64	32	8	2	16	128	0	0
256	1024^3	1.077	8	8	2	2	4	16	16	2	4	8	32	7	4	2	1	16	8	4	2	2	8	32	0	0
512	1024^3	0.567	32	4	2	2	8	16	8	2	16	4	8	5	2	2	2	4	16	8	1	8	4	8	0	0
1024	1024^3	0.292	64	4	2	1	8	16	8	1	8	8	16	4	8	4	2	8	64	8	2	4	4	32	0	0
2048	1024^3	0.272	64	4	1	2	4	64	8	4	2	8	8	3	4	3	1	2	32	16	2	4	8	16	0	0
4096	1024^3	0.167	16	32	0	2	2	0	0	8	4	0	0	1	4	0	2	32	0	0	4	4	0	0	0	1
8192	1024^3	0.125	8	128	0	32	1	0	0	2	1	0	0	8	1	0	1	64	0	0	1	16	0	0	0	0
16384	1024^3	0.062	64	16	0	2	2	0	0	8	2	0	0	4	4	0	1	4	0	0	2	2	0	0	0	0
32768	1024^3	0.049	128	8	0	4	2	0	0	2	2	0	0	3	4	0	2	4	0	0	2	2	0	0	0	1

(c) Edison (Weak Scaling)

p	N_x	N_y	N_z	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
128	512	512	512	0.114	1	8	4	1	2	32	16	2	1	16	16	X	X	X	X	X	X	X	X	X	X	X	0	1
256	512	512	1024	0.139	1	32	5	1	2	32	32	1	2	32	32	X	X	X	X	X	X	X	X	X	X	X	0	1
512	1024	1024	512	0.155	1	64	4	32	1	128	4	2	1	32	64	X	X	X	X	X	X	X	X	X	X	X	0	1
1024	1024	1024	1024	0.159	64	4	2	2	32	4	2	2	2	4	8	5	16	1	4	8	32	8	4	4	8	32	0	0
2048	1024	1024	2048	0.190	128	1	4	1	64	4	1	1	64	2	16	3	64	1	8	8	256	8	2	8	16	32	0	0
4096	2048	2048	1024	0.202	256	2	1	1	128	16	2	2	1	8	128	7	4	4	2	2	32	8	1	4	8	32	0	0
8192	2048	2048	2048	0.207	512	2	1	1	16	64	4	1	4	4	16	1	16	2	8	2	64	8	4	2	16	64	0	0
16384	2048	2048	4096	0.288	1024	2	0	1	32	0	0	2	1	0	0	2	64	3	1	1	128	128	4	2	16	128	0	0
32768	4096	4096	2048	0.341	256	4	2	1	4	64	32	4	8	2	32	9	8	1	2	8	64	8	1	16	8	64	0	0

(d) Hopper (Weak Scaling)

p	N_x	N_y	N_z	time(s)	D	T_1	W_1	P_{x1}	P_{y1}	F_z	F_{p1}	U_{x1}	U_{z1}	F_{u1}	F_{y1}	R_y	T_2	W_2	P_{z2}	P_{x2}	F_{y2}	F_{p2}	U_{z2}	U_{y2}	F_{u2}	F_x	V	S
128	512	512	512	0.243	1	128	1	2	2	256	32	8	1	64	512	X	X	X	X	X	X	X	X	X	X	X	0	0
256	512	512	1024	0.274	16	8	1	2	32	4	4	1	2	4	64	5	2	4	1	16	8	4	1	8	8	4	0	0
512	1024	1024	512	0.283	64	4	2	1	32	64	2	2	2	2	16	1	8	1	2	16	16	4	1	2	16	128	0	0
1024	1024	1024	1024	0.292	64	4	2	1	8	16	8	1	8	8	16	4	8	4	2	8	64	8	2	4	4	32	0	0
2048	1024	1024	2048	0.445	128	2	1	1	8	32	4	1	8	4	16	3	32	0	8	4	0	0	4	4	0	0	0	0
4096	2048	2048	1024	0.516	256	4	1	2	8	16	8	2	4	8	16	6	16	0	2	1	0	0	2	4	0	0	0	0
8192	2048	2048	2048	0.612	512	2	1	2	32	2	4	2	16	4	128	0	16	0	4	2	0	0	16	4	0	0	0	0
16384	2048	2048	4096	0.996	1024	2	0	2	8	0	0	1	4	0	0	2	64	1	4	2	128	32	2	2	64	128	0	0
32768	4096	4096	2048	1.121	512	2	2	2	4	32	8	1	4	4	32	6	16	1	4	2	64	32	2	4	16	64	0	0

(a) Edison (Strong Scaling)

(b) Hopper (Strong Scaling)

(c) Edison (Weak Scaling)

(d) Hopper (Weak Scaling)

Figure 6: Parallel 3-D FFT Speedup of NEW Relative to Other Algorithms on Large Scale Experiments: We used all 24 cores per node of Edison and Hopper. Strong scaling fixes an input size at 1024^3 elements. Weak scaling doubles an input size from 512^3 through $4096 \times 4096 \times 2048$. NEW shows speedup of up to $1.35\times$ over FFTW, $2.57\times$ over DCMP, and $1.36\times$ over UPCF on Edison. The speedup on Hopper is up to $1.32\times$ over FFTW, $1.77\times$ over DCMP, and $1.95\times$ over UPCF.

Pack2+Unpack2) of NEW is longer than communication time (Wait2) of NEW-0. We conjecture that the reason of non-optimized overlap on Hopper comes from memory access contention. Since we use all 24 cores per node, the communication of each core makes slow progress as it contends with memory access operations of other cores. We have a better overlap on Edison because Edison is a newer machine with higher memory bandwidth and larger L3 caches.

5.2.2. The Necessity of Auto-Tuning

Table 2 contains the auto-tuned parameter configurations of NEW. We can see that the best parameter values vary depending on system settings such as platform, input size, and the number of cores. Figure 10(a) shows the history of an auto-tuning execution for the setting of $p = 512$ and $N^3 = 1024^3$. The x -axis means the tuning step number. The y -axis means the 3-D FFT time for the

parameter configuration found at each tuning step. The execution time decreases as the tuning proceeds. There is around $10\times$ performance gap between the best and the worst configurations. Thus we should tune the parameters properly to achieve high performance of 3-D FFT.

We conducted cross-platform tests to further explore the necessity of auto-tuning. We executed the 3-D FFT code on Edison with a cross-platform parameter setting that uses the tuning result from Hopper (Table 2(b)). CRSS in Figure 5(a) shows the speedup of the original setting over this cross-platform setting. The original setting is always faster (by up to $1.43\times$) than the cross-platform settings. Likewise, we have executed the 3-D FFT code on Hopper with the tuning result of Edison as shown in Table 2(a). CRSS in Figure 5(b) shows the speedup of NEW (up to $2.54\times$) on Hopper relative to the cross-platform setting from Edison. The best configura-

(a) Edison (Strong Scaling)

(b) Hopper (Strong Scaling)

(c) Edison (Weak Scaling)

(d) Hopper (Weak Scaling)

Figure 7: Parallel 3-D FFT Execution Time on Large Scale Experiments (log-log Scale Plot): Strong scaling fixes an input size at 1024^3 elements. Weak scaling doubles an input size from 512^3 through $4096 \times 4096 \times 2048$. NEW scales up to at least 32,768 cores while FFTW only scales up to 1,024 cores.

tion for Edison is not the best on Hopper, and vice versa. Thus, it is necessary to auto-tune our 3-D FFT code for each different platform to achieve the best of its performance.

5.3. Large Scale Experiments

For strong scaling experiments, we increase p from 128 through 32,768 cores (around a quarter of the total cores), and we have a fixed-size input array with 1024^3 elements. The third column of Table 3(a) shows the 3-D FFT execution time of our NEW approach on Edison. Figure 6(a) shows the speedup of our NEW approach relative to three other approaches on Edison. NEW shows speedup of up to $1.29\times$ over FFTW, $2.57\times$ over DCMP, and $1.36\times$ over UPCF. Note that FFTW only scales up to 1,024 cores as FFTW is based on 1-D decomposition. On the other hand, NEW, DCMP, and UPCF scale to at least 32,768 cores as they are all based on 2-D decomposition. Figures 7(a)

and 8(a) show the parallel 3-D FFT execution time and the FLOPS performance for strong scaling experiments on Edison. The execution time of NEW decreases from 0.965 seconds to 0.012 seconds. We also computed FLOPS performance values based on the rule of $5N \log_2 N$ floating point operations for 1-D FFT on N elements. [9] The FLOPS performance of NEW ranges from 167 GFLOPS to 13,603 GFLOPS, which means the parallel efficiency is 31.8% going from 128 to 32,768 cores. The strong scaling performance increases sub-linearly as parallel 3-D FFT involves heavy overhead of global communication patterns at large p .

In weak scaling experiments, p increases from 128 to 32,768 cores, and the input size also doubles from 512^3 through $4096 \times 4096 \times 2048$. The fifth column of Table 3(c) shows the 3-D FFT execution time of NEW on Edison. Figures 6(c), 7(c), and 8(c) show the results of weak scaling experiments on Edison. The speedup of NEW

(a) Edison (Strong Scaling)

(b) Hopper (Strong Scaling)

(c) Edison (Weak Scaling)

(d) Hopper (Weak Scaling)

Figure 8: Parallel 3-D FFT Performance in GFLOPS on Large Scale Experiments (log-log Scale Plot): Strong scaling fixes an input size at 1024^3 elements. Weak scaling doubles an input size from 512^3 through $4096 \times 4096 \times 2048$. NEW achieves 13,603 GFLOPS (strong scaling) and 17,611 GFLOPS (weak scaling) at 32,768 cores on Edison. The performance of NEW on Hopper is 3,262 GFLOPS (strong scaling) and 5,365 GFLOPS (weak scaling) at 32,768 cores.

is up to $1.35\times$ over FFTW, $1.26\times$ over DCMP, and $1.34\times$ over UPCF. The FFT execution time of NEW increases from 0.114 seconds to 0.341 second. The curves in Figure 7(c) are increasing with p while they are supposed to be flat in the ideal weak scaling. One reason of the non-flat curve is the overhead of all-to-all communication. The other reason is because the computation complexity of 3-D FFT grows faster than an input size. For an input with $N_x \times N_y \times N_z$ elements, we need $O(N_x N_y N_z \log(N_x N_y N_z))$ floating point operations. The FLOPS performance of NEW ranges between 159 GFLOPS and 17,611 GFLOPS, which means the parallel efficiency is 43.3% going from 128 to 32,768 cores. The parallel efficiency of weak scaling is higher than strong scaling because weak scaling has less communication overhead with larger-size messages than strong scaling.

Likewise, we did the same experiments for strong scal-

ing and weak scaling on Hopper. Table 3(b) and Figures 6(b), 7(b), and 8(b) show the results of strong scaling experiments on Hopper. NEW shows speedup of up to $1.32\times$ over FFTW, $1.77\times$ over DCMP, and $1.66\times$ over UPCF. (UPCF crashed at 16,384 and 32,768 cores after producing an unknown error.) The execution time of NEW decreases from 1.673 seconds to 0.049 seconds. The FLOPS performance increases from 96 GFLOPS to 3,262 GFLOPS, which means the parallel efficiency is 13.2% going from 128 to 32,768 cores. Table 3(d) and Figures 6(d), 7(d), and 8(d) show the results of weak scaling experiments on Hopper. NEW shows speedup of up to $1.11\times$ over FFTW, $1.42\times$ over DCMP, and $1.95\times$ over UPCF. (UPCF crashed at 32,768 cores after producing an unknown error.) The execution time of NEW increases from 0.243 seconds to 1.121 second. The FLOPS performance increases from 75 GFLOPS to 5,365 GFLOPS, which means the parallel

(a) Small Scale ($p = 512$, $N^3 = 1024^3$)

(b) Large Scale ($p = 32768$, $N_x \times N_y \times N_z = 4096 \times 4096 \times 2048$)

Figure 9: Execution Time Breakdown: NEW-0 is a non-overlapped version of NEW. The difference of the Wait1 and Wait2 time between NEW-0 and NEW means the all-to-all communication time overlapped with computation.

(a) Small Scale ($p = 512$, $N^3 = 1024^3$)

(b) Large Scale ($p = 32768$, $N_x \times N_y \times N_z = 4096 \times 4096 \times 2048$)

Figure 10: Auto-Tuning History on Edison: The 3-D FFT time for a test parameter configuration decreases as the tuning proceeds. There is around 10 $\times$ performance gap between the best and the worst configurations. Thus we should tune the parameters properly to achieve high performance of 3-D FFT.

efficiency is 28.1% going from 128 to 32,768 cores.

In large-scale experiments, NEW is still faster than FFTW, DCMP, and UPCF for almost all different input settings. As we discussed in the previous section, the successful computation-communication overlap is the reason of NEW's high performance. For example, Figure 9(b) shows the breakdown of the execution time of NEW for the $p = 32768$ and $N_x \times N_y \times N_z = 4096 \times 4096 \times 2048$ configuration. On Edison and Hopper, NEW reduces communication time (Wait1 and Wait2) compared to the non-overlapped version NEW-0. Table 3 contains the auto-tuned parameter configurations of NEW, which shows that the best parameter values vary depending on system settings. Figure 10(b) shows the history of an auto-tuning execution for one setting on Edison. There is around 10 $\times$ performance gap between the best and the worst configu-

rations. We could achieve high performance of 3-D FFT in large-scale experiments by utilizing the auto-tuning technique.

The FFT performance on Edison is faster than Hopper for all input settings. Edison is a newer machine with faster inter-connection network and higher computation performance than Hopper. Also, the parallel efficiency on Edison is higher than Hopper. The Dragonfly network of Edison [18, 19] connects compute nodes with short hop distances which is beneficial for all-to-all communication, and the dynamic routing mechanism balances network traffic over inter-connection links. Thus Edison handles large-scale global network traffic better than the 3-D Torus network of Hopper.

5.4. Tuning Costs

In order to quantify the cost of auto-tuning, we collected all the history of 270 auto-tuning executions of NEW that generated the results in Tables 2 and 3. Figure 11 shows the distribution of the number of tuning steps taken by each tuning execution. y -axis means the cumulative fraction of tuning executions, and x -axis represents the number of tuning steps. The curve marked with “converge” represents the distribution of the total number of tuning steps that each tuning execution takes until the Nelder-Mead algorithm converges. The curve marked with “best” represents the distribution of the number of tuning steps that each tuning execution takes until finding the best configuration. Figure 11 shows that our method uses 121 steps until convergence in the median case ($y = 0.5$), and the best configuration is found after 92 steps. Note that scientific simulations normally execute more than tens of thousands of time steps, each of which involves a couple of 3-D FFT operations. Thus our auto-tuning cost of around 100 3-D FFT operations will be almost negligible in such scientific simulations. This low cost of tuning is the result of our customization techniques described in Section 4.3.

Despite the already low tuning cost, we can reduce it even more by sacrificing a little bit of 3-D FFT performance. The other curves in Figure 11 represent the number of tuning steps that each tuning execution takes until finding a configuration close to the best one. For example, the curve of “5% worse” is for a configuration such that the 3-D FFT time takes 5% more than the best configuration. It is interesting that we can still find a good configuration by shortening many tuning steps. For example, we can find a “5% worse” configuration after 41 steps (median), which is faster than 92 steps for the “best” configuration by more than a factor of two. Thus we can bring down the 3-D FFT performance slightly and shorten the number of tuning steps significantly.

6. Related Work

FFTW [9] does not overlap any computation with communication, so it results in the poor performance of 3-D FFT as shown in Section 5. Also, FFTW is not scalable as it is designed based on 1-D decomposition. P3DFFT [4], 2DECOMP&FFT [5], Ayala et al. [6], Takahashi [7], and Eleftheriou et al. [20] achieved high scalability with the high-dimensional domain decomposition technique. However, they did not include any overlap between computation and communication. On the other hand, our approach increases both of the performance and scaling through computation-communication overlap and 2-D decomposition.

Doi et al. [21] overlap computation and communication in a shared-memory parallel environment. However, each core uses blocking communication, and the overlap takes place between cores. On the other hand, we exploit non-blocking communication for the overlap within

Figure 11: Cumulative Distribution of the Number of Tuning Steps: In the median case ($y = 0.5$), the “best” configuration is found after 92 steps, which is almost negligible in scientific simulations executing more than tens of thousands of 3-D FFT operations. We can reduce the tuning cost significantly by sacrificing a little bit of 3-D FFT time. For example, a “5% worse” configuration is found after 41 steps.

each core. Bell et al. [13] and Nishtala et al. [8] wrote a UPC-based code that requires hardware support for asynchronous communication. As shown in Section 5, the UPC-based code is not optimized because 1) it misses some computation to overlap with communication, 2) it uses a fixed size of communication messages, and 3) it uses the point-to-point communication rather than the optimized collective operation. Fang et al. [22] lack portability as they use a special communication API called QMP and require hardware support for asynchronous communication. Also, there is no auto-tuning of overlap-related parameters. Similarly to our approach, Hoefer et al.’s work [10] and our previous work [11] succeeded in using `MPI_Ialltoall` for 3-D FFT, but they have limitations on scalability as they are based on 1-D decomposition. Note that our algorithm also supports 1-D decomposition through auto-tuning.

Kandalla et al. [23] overlap the computation on one input array with the communication for other arrays. This “inter-array” overlap is useful when there are many independent arrays for 3-D FFT. However, scientific simulations [1] normally need successive 3-D FFT computations over time on a single array. In this case, our “intra-array” method is effective as we overlap computation with communication inside each 3-D FFT operation. Also, Kandalla et al.’s approach requires hardware support for asynchronous communication.

7. Conclusions and Future Work

This paper presented a scalable method for parallel 3-D FFT that exploits computation-communication overlap. Our work is the first to effectively apply non-blocking MPI collectives to the 2-D decomposition method for parallel

3-D FFT. We need no special hardware support for asynchronous communication. We also described a method to auto-tune our 3-D FFT code in a large parameter space. Experimental results show that our code scales well up to at least 32,768 cores, and performs faster than three other approaches including the UPC-based code. Our auto-tuning technique is effective as two systems require different settings of the best parameter configuration.

We are planning to extend this work by improving the auto-tuning method. The quality and speed of the Nelder-Mead heuristic is dependent on how the initial simplex is defined. Although our definition of the initial simplex was successful, it is worth investigating if there exist other more effective initial simplex construction techniques. Also, we plan to try optimization strategies other than Nelder-Mead.

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