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Performance modeling of hybrid MPI/OpenMP scientific applications on large-scale multicore supercomputers

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ABSTRACT

In this paper, we present a performance modeling framework based on memory bandwidth contention time and a parameterized communication model to predict the performance of OpenMP, MPI and hybrid applications with weak scaling on three large-scale multicore supercomputers: IBM POWER4, POWER5+ and BlueGene/P, and analyze the performance of these MPI, OpenMP and hybrid applications. We use STREAM memory benchmarks and Intel's MPI benchmarks to provide initial performance analysis and model validation of MPI and OpenMP applications on these multicore supercomputers because the measured sustained memory bandwidth can provide insight into the memory bandwidth that a system should sustain on scientific applications with the same amount of workload per core. In addition to using these benchmarks, we also use a weak-scaling hybrid MPI/OpenMP large-scale scientific application: Gyrokinetic Toroidal Code (GTC) in magnetic fusion to validate our performance model of the hybrid application on these multicore supercomputers. The validation results for our performance modeling method show less than 7.77% error rate in predicting the performance of hybrid MPI/OpenMP GTC on up to 512 cores on these multicore supercomputers.

1. Introduction

Today, the trend in high performance computing systems has been shifting towards cluster systems with multicore. Further, multicore processors are usually configured hierarchically (e.g., multiple multicores compose a multi-chip module to form a node) to form a compute node of parallel systems. While multicore presents significant new opportunities such as on-chip high inter-core bandwidth and low latency, it also presents new challenges in the form of inter-core resource conflict and contention. For many years, there has been considerable concern over the growing imbalance between memory subsystem performance and processor performance. Many of us fear that multicore continues to exacerbate memory bandwidth problems, however, the stall in processor frequency has diminished the corresponding worsening of memory latency in terms of processor-clocks [11].

Levesque et al. [11] observed from the AMD architectural discussion that when excluding messaging performance, the primary source of contention when moving from single core to dual core is memory bandwidth, and confirmed this assumption by the testing with STREAM [12] and Membench microbenchmarks. In our previous work [20,19,18], we also found that memory bandwidth contention is the primary source of performance degradation for L2/L3 shared architectures such as CrayXT4/XT5 and IBM Power4/Power5 and BlueGene/P systems using NAS parallel benchmarks and large-scale scientific

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Table 1
Specifications of three multicore supercomputers.

Configurations	BlueGene/P (Intrepid)	P655	Hydra
Number of nodes	40,960	272	40
Number of cores	163,840	2176	640
Cores/chip	4	2	2
Cores/node	4	8	16
CPU type	1.9 GHz	1.5, 1.7 GHz	850 MHz PowerPC
Memory/node	2 GB	16, 32 GB	32 GB
L1 cache/CPU	32 KB	64/32 KB	64/32 KB
L2 cache/chip	16 128 B lines	1.41 MB	1.92 MB
L3 cache/chip	8 MB	32 MB	36 MB
Network	3D torus	Federation	Federation

applications such as the Gyrokinetic Toroidal Code (GTC) [7] when increasing the number of cores per node. Therefore, in this paper, we focus on scientific applications with memory bandwidth contention problems, and present a performance modeling framework based on memory bandwidth contention time on small number of cores to predict the performance on larger number of cores.

Multicore supercomputers provide a natural programming paradigm for hybrid MPI/OpenMP applications. Current hybrid parallel programming paradigms such as hybrid MPI/OpenMP need to efficiently exploit the potential offered by such multicore supercomputers. Generally, MPI is considered optimal for process-level coarse parallelism and OpenMP is optimal for loop-level fine grain parallelism. Combining MPI and OpenMP parallelization to construct a hybrid program is not only to achieve multiple levels of parallelism but also to reduce the communication overhead of MPI at the expense of introducing OpenMP overhead due to thread creation and increased memory bandwidth contention. In this paper, we analyze the performance of MPI, OpenMP and hybrid applications on three large-scale multicore supercomputers: IBM POWER4, POWER5 and BlueGene/P, and present a performance modeling framework based on memory bandwidth contention time and parameterized communication model to predict the performance of OpenMP, MPI and hybrid applications with weak scaling on these multicore supercomputers.

The experiments conducted for this work utilize multicore supercomputers with different number of cores per node. P655 [14] has 8 cores per node, Hydra [15] has 16 cores per node, and BlueGene/P (Intrepid) [3] at Argonne National Laboratory (ANL) has 4 cores per node. Further, each system has a different node memory hierarchy. We use the MPI and OpenMP STREAM memory benchmarks [12] and Intel's MPI benchmarks [9] to provide initial performance analysis of MPI and OpenMP applications on these multicore supercomputers. In addition to using these benchmarks, we also use a hybrid MPI/OpenMP large-scale scientific application: a 3D particle-in-cell application GTC in magnetic fusion to validate our performance models of these MPI, OpenMP and hybrid applications. Our experimental results for our performance modeling method show less than 7.77% error rate in predicting the performance of MPI, OpenMP and hybrid MPI/OpenMP GTC on up to 512 cores of these multicore supercomputers.

The remainder of this paper is organized as follows. Section 2 discusses the architecture and memory hierarchy of three large-scale multicore supercomputers used in our experiments, and compares their performance using STREAM benchmarks and Intel's MPI benchmarks. Section 3 proposes and discusses a performance modeling framework for hybrid MPI/OpenMP applications based on memory bandwidth contention time and a parameterized communication model. Section 4 validates our performance models using the hybrid GTC. Section 5 discusses some related work and Section 6 concludes this paper. In the remainder of this paper, we assume that the job scheduler for each multicore supercomputer always dispatches one process to one core or one thread to one core. We describe the system configuration as $M \times N$ whereby M denotes the number of nodes with N cores per node. All experiments were executed multiple times to ensure consistency of the performance data. Prophesy system [16] is used to collect all application performance data.

2. Execution platforms and performance

In this section, we briefly describe three large-scale multicore supercomputers used for our experiments, use Intel's MPI Benchmark Ping Pong [9] to measure and compare MPI bandwidth and latency, and use MPI and OpenMP STREAM memory benchmarks [12] to measure and compare sustainable memory bandwidth for MPI and OpenMP programs on these multicore supercomputers.

2.1. Descriptions of execution platforms

Details about three large-scale multicore supercomputers used for our experiments are given in Table 1. These supercomputers differ in the following main features: number of cores per node, configurations of node memory hierarchy, CPU speed, multicore processors, operating systems, and communication networks.

BlueGene/P (Intrepid) at Argonne Leadership Computing Facility [3] at Argonne National Laboratory is an IBM BlueGene/P supercomputer with 40,960 quad-core nodes and 80 terabytes of memory. Its computer nodes are each connected

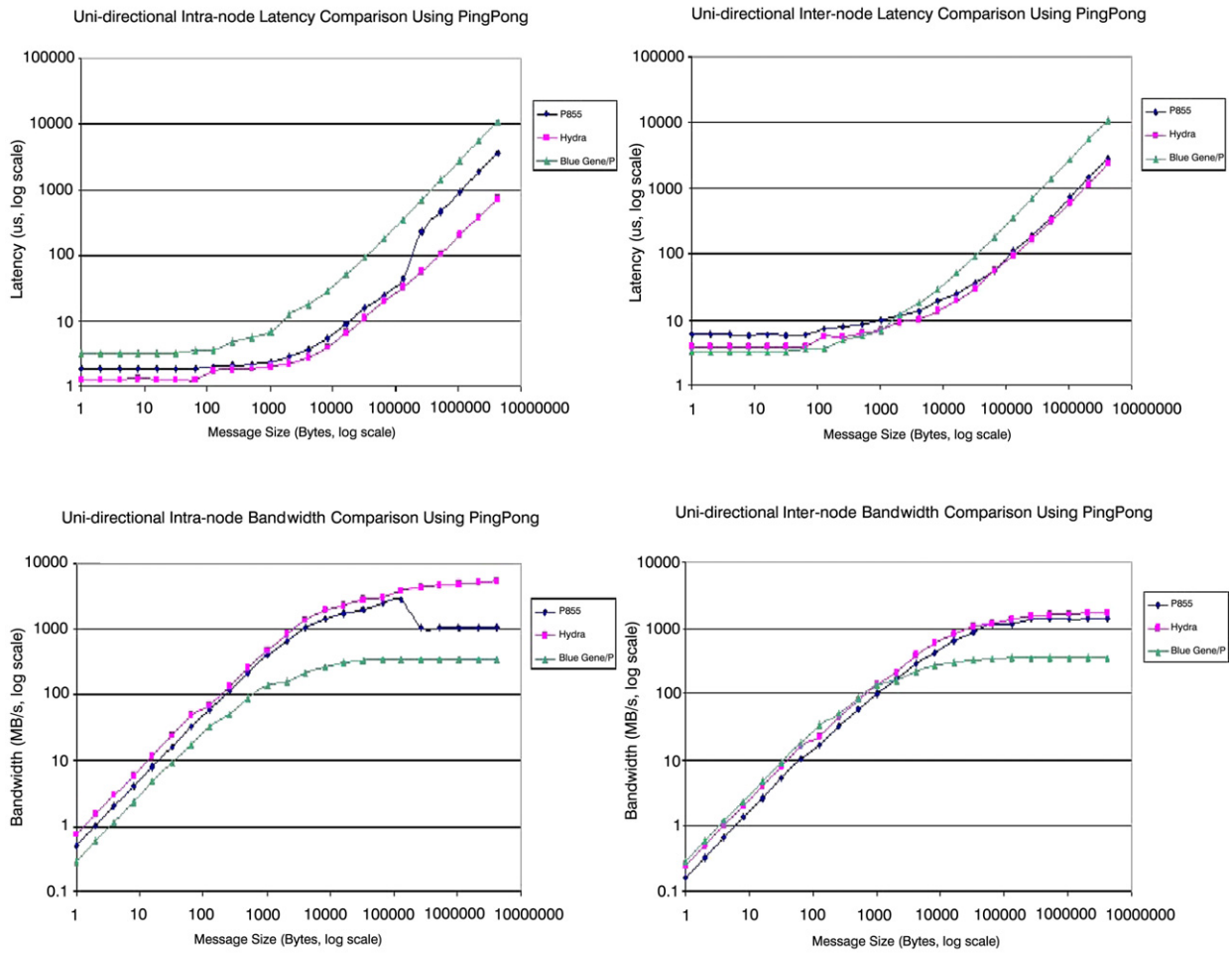

Fig. 1. Uni-directional intra/inter-node latency and bandwidth comparison using PingPong.

to multiple inter-node networks, including a high-performance, low-latency 3D torus, a highly scalable collective network, and a fast barrier network.

SDSC DataStar P655 [14] is an IBM POWER4 supercomputer with 176 (8-way) compute nodes with 1.5 GHz POWER4 and 16 GB memory, and 96 (8-way) compute nodes with 1.7 GHz POWER4 and 32 GB memory. Each node of P655 has one MCM (multiple-chip module) with 4 chips per MCM. The use of 8-way nodes for P655 is exclusive.

Hydra at Texas A&M University Supercomputer Facility [15] is an IBM POWER5+ supercomputer with 40 POWER5-575 nodes, and each node has 32 GB of memory and 8 DCMs (dual-chip modules) with a dual-core POWER5+ processor per DCM.

2.2. MPI bandwidth and latency comparison

In this section, we use Intel's MPI benchmark PingPong [9] to measure uni-directional point-to-point performance between two processes within the same node (one process per processor) for intra-node performance (memory performance), and between two nodes (one process per node) for inter-node performance (network performance). The results shown in Fig. 1 indicate almost doubling of the latency and a significant reduction in bandwidth when going from communication within a node to communication between nodes using PingPong on P655 and Hydra, however, inter-/intra-node latency and bandwidth on BlueGene/P remain almost the same because of 3D torus network connection. The bandwidth for BlueGene/P also remains flat for message sizes of 128 KB or larger. The MPI intra-node bandwidth on BlueGene/P is much smaller than that on other multicore supercomputers.

2.3. Sustainable memory bandwidth comparison

In this section, we use the MPI and OpenMP versions of the STREAM memory benchmark [12] to investigate memory performance for different system configurations.

Table 2
Sustainable memory bandwidth on P655.

Program type	MPI				OpenMP
Configuration	1×8	2×4	4×2	8×1	8 threads
Memory bandwidth (MB/s)	16106.13	20132.66	26843.55	40265.32	18249.16

Table 3
Sustainable memory bandwidth on Hydra.

Program type	MPI					OpenMP
Configuration	1×16	2×8	4×4	8×2	16×1	16 threads
Memory bandwidth (MB/s)	32212.25	53687.09	80530.64	80530.64	80530.64	57063.45

Table 4
Sustainable memory bandwidth on BlueGene/P.

Program type	MPI			OpenMP
Configuration	1×4	2×2	4×1	4 threads
Memory bandwidth (MB/s)	16106.13	16106.13	16106.13	8977.32

The STREAM benchmark is a synthetic benchmark program, written in standard Fortran 77 and MPI for MPI version and in C and OpenMP for OpenMP version. It measures the performance of four long vector operations (double precision): COPY (i.e., $a(i) = b(i)$), SCALE (i.e., $a(i) = q * b(i)$), SUM (i.e., $a(i) = b(i) + c(i)$), and TRIAD (i.e., $a(i) = b(i) + q * c(i)$), and it is specifically intended to eliminate the possibility of data re-use (either in registers or caches). The TRIAD allows chained/overlapped/fused multiple/add operations. In this paper, we only use unit-stride TRIAD benchmark to measure the sustainable memory bandwidth. We find that most multicore supercomputers we used only support array sizes of at most 4M (2^{22}) with 8 bytes per double precision word because of lack of sufficient memory to start the benchmark. So we set the array size 4M for MPI and OpenMP STREAM benchmarks.

Because P655 has 8 cores per node, so we use STREAM benchmarks to measure the sustainable bandwidths on 8 cores. For different configurations using processor partitioning [17,18], Table 2 shows the sustainable memory bandwidth increases from 16106.13 MB/s to 40265.32 MB/s with decreasing the number of cores per node from 8 cores per node to 1 core per node for using 8 MPI processes because fewer MPI processes compete for memory. We see that the sustainable memory bandwidth for using 8 OpenMP threads is larger than that for using 8 MPI processes with the configuration 1×8, but smaller than the others because of the memory contentions.

Table 3 shows the memory bandwidths for three configurations 16×1, 8×2 and 4×4 are the same on Hydra. These memory bandwidths are more than two times larger than that for the configuration 1×16. We also see that the sustainable memory bandwidth for using 16 OpenMP threads is larger than that for using 16 MPI processes with the configuration 1×16.

Table 4 indicates no difference in memory bandwidths for difference configurations on BlueGene/P, and the memory bandwidth for using 4 OpenMP threads is almost half less than that for using 4 MPI processes.

In summary, Tables 2, 3, and 4 present the sustainable memory bandwidths for MPI and OpenMP on the three multicore supercomputers. For all these systems, different system configurations impact the sustainable memory bandwidth. Hence, using fewer cores per node results in better sustainable memory bandwidth, and except on BlueGene/P, using the maximum number of cores per node never resulted in the highest sustainable memory bandwidth.

3. Performance models for hybrid MPI/OpenMP scientific applications

In this section, we propose a performance modeling framework based on memory bandwidth contention time and a parameterized communication model, and use the performance modeling framework to model and predict the performance of OpenMP, MPI and hybrid applications.

3.1. Performance models for OpenMP applications

Fig. 2 illustrates a simple OpenMP multithread process, where the program consists of sequential components S1 and S2 and parallelized components P1, P2, P3 and P4. The OpenMP program proceeds in the fork–join-like model. First, it processes S1, then the master thread (the process itself) forks three threads. The four threads process P1, P2, P3 and P4 in parallel. When they are finished, they are joined to the master thread. Then the program processes S2. Note that there is some overhead in forking and joining OpenMP threads. Since all the OpenMP threads belong to a single process, they share the same address space and it is easy to reference data that other threads have updated.

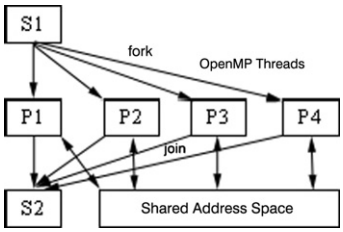

Fig. 2. One multithreads process.

As discussed above in Section 2.3, Tables 2, 3, and 4 indicate that sustainable memory bandwidth decreases with increasing number of processors per node except that on BlueGene/P. The experimental results also indicate that the application execution time decreases with increasing the number of processors per node [17]. In [20,19,18], we found that memory bandwidth contention is the primary source of performance degradation for L2/L3 shared architectures when increasing the number of processors per node.

In [11], the primary source of contention when moving from single core to dual core on AMD Opteron architecture is memory bandwidth, and a simple performance model for a sequential program was proposed to extrapolate the quad-core performance by assuming the time spent in the execution component remains the same, but the time spent in memory bandwidth contention will increase proportional to the reduction in effective memory bandwidth per core. In this section, we generalize the performance model to support parallel applications (OpenMP, MPI or hybrid) to extrapolate the performance of the multicore node (which consists of one or several multicores) by enumerating the following assumptions of our model:

(i) The primary source of performance difference between single- and multi-core runs is memory bandwidth contention when excluding message passing performance.
(ii) Computation time of a parallel program can be broken into the portion that is stalled on shared resources (memory bandwidth) and the portion that is stalled on non-shared resources.
(iii) For an application with a fixed workload per processor core, assume that the time spent in the computation component per core (T_C) remains the same, however, the time spent in memory bandwidth contention (T_M) will increase proportional to the reduction in effective memory bandwidth per core.

The assumption (i) was confirmed in [11,20,19,18], which means that our focus is on scientific applications with memory bandwidth contention problems. I/O performance is not considered in these kinds of applications. The assumption (ii) is consistent to that CPU execution time equals CPU time plus memory stall time defined by Hennessy and Patterson [8].

The assumption (iii) was confirmed in [18–20], especially in [18], when excluding message passing performance, the decrease percentage for the bandwidth of the data traffic between memory and D1 cache, between L2 and D1 cache or between L2 and memory is similar to the increase percentage for the total execution times of eight NAS parallel benchmarks with classes B and C when using from 1 core per node, 2 cores per node to 4 cores per node, where the workload per core remains the same.

If the assumptions above hold true, we expect execution time to obey the following relationships:

$$T_1 = T_C + T_M \quad \text{and} \quad T_2 = T_C + \gamma_2 T_M \tag{1}$$

Here T_1 and T_2 denote the execution time on one core and two cores, respectively; γ_2 denotes memory bandwidth ratio which is the memory bandwidth for the baseline (one core) divided by the memory bandwidth for the target (two cores). ($\gamma_2 > 1$ because of memory bandwidth contention. We use the STREAM memory benchmark to measure the sustained memory bandwidths on one or two cores to calculate the memory bandwidth ratio.) From Eq. (1), we have

$$T_M = \frac{T_2 - T_1}{\gamma_2 - 1} \quad \text{and} \quad T_C = T_1 - \frac{T_2 - T_1}{\gamma_2 - 1} \tag{2}$$

We can use Eq. (2) to predict the execution time T_4 on four cores as follows. Assume that γ_4 denotes memory bandwidth ratio, which is the memory bandwidth for the baseline (one core) divided by the memory bandwidth for the target (four cores). From the assumption (iii), we have

$$T_4 = T_C + \gamma_4 T_M \tag{3}$$

From Eqs. (2) and (3), we have the execution time on four cores

$$T_4 = \left(T_1 - \frac{T_2 - T_1}{\gamma_2 - 1}\right) + \gamma_4 \frac{T_2 - T_1}{\gamma_2 - 1} = T_1 + (\gamma_4 - 1)\frac{T_2 - T_1}{\gamma_2 - 1} \tag{4}$$

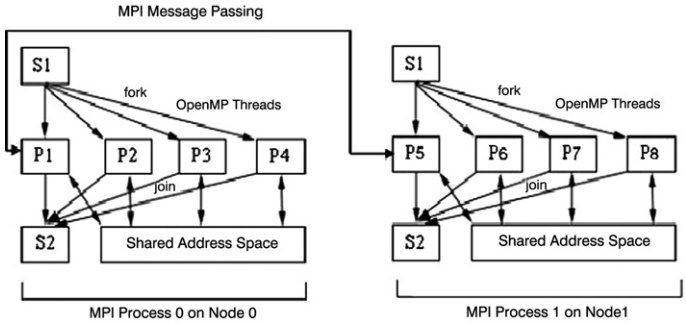

Fig. 3. One multithreads process per node.

This demonstrates how to use the performance model based on performance data on one core or two cores to predict the performance on four or more cores. Note that the assumption (iii) means that the performance model is only for weak-scaling applications where the time spent in the computation component per core remains the same. The memory bandwidth ratios γ_2 and γ_4 for OpenMP applications are only measured once, then can be used for modeling any OpenMP applications on the system. We can generalize Eq. (4) to a general case for using n cores.

Assume that γ_n denotes memory bandwidth ratio, which is the memory bandwidth for the baseline (one core) divided by the memory bandwidth for the target (n cores). From Eq. (4), we have the general model for the application execution time on n cores

$$T_n = T_C + \gamma_n T_M = \left(T_1 - \frac{T_2 - T_1}{\gamma_2 - 1}\right) + \gamma_n \frac{T_2 - T_1}{\gamma_2 - 1} = T_1 + (\gamma_n - 1)\frac{T_2 - T_1}{\gamma_2 - 1} \tag{5}$$

This equation indicates that, given the fixed workload per core, the equation is used to predict the application performance on n cores based on the performance for single and dual cores and the memory bandwidth ratios for dual (γ_2) and many cores (γ_n), where the memory bandwidth ratios are associated with the sustained memory bandwidths on 1, 2 and n cores, which provide insight into the memory bandwidth that a system should sustain on various classes of scientific applications. Therefore, this performance model will be helpful to understand the application performance on multi- and many cores. The performance modeling method for OpenMP applications can also be applied to computation components of an MPI program for the given problem size and number of cores.

Given problem size and number of cores, using processor partitioning [17,18], we measure the sustainable memory bandwidths for MPI STREAM memory benchmark on three multicore supercomputers, P655, Hydra, and BlueGene/P as shown in Tables 2–4, then use them to calculate the memory bandwidth ratio γ_2 and γ_4 (the baseline bandwidth for using one core per node). Assume that T_1 and T_2 denote the computation times of an MPI program for using one core per node and two cores per node, respectively. Because of using processor partitioning for the given number of cores, the time spent in the computation component per core remains the same. Therefore, we can use Eq. (4) to predict the computation time of the MPI program for using four cores per node. For communication component of the MPI program, we can parameterize the communication component based on each MPI subroutine to generate a parameterization model. We will discuss the communication parameterization model in detail in the following section (Section 3.2).

3.2. Performance models for hybrid MPI/OpenMP applications

For hybrid MPI/OpenMP applications, modeling their performance is more complicated because of so many different combinations of MPI processes and OpenMP threads. In previous work [19], for the MPI GTC, we found that using fewer processors per node resulted in the better performance, and using one processor per node resulted in the best performance for the MPI version of GTC. In this section, for the sake of simplicity, we consider using one MPI process per node and one OpenMP thread per core on each node to model the performance of the hybrid applications executed on these multicore supercomputers. In other words, for the execution of a hybrid application, MPI is used for internode communication, and OpenMP is used for intranode communication.

Fig. 3 illustrates one simple OpenMP-multithread MPI process per node. To utilize the shared memory feature of multicore nodes, we run one MPI process with OpenMP multithreads on each node so that intranode communication uses shared memory and internode communication uses message passing. This can take advantage of inter-core high bandwidth and low latency provided by multicore. As shown in Fig. 3, the hybrid program is an SPMD (Single Program Multiple Data) program. The program execution consists of two MPI processes with four OpenMP threads per MPI process. For instance, inside each node (node 0 or node 1), shared address space is used for data exchange among OpenMP threads. MPI message passing is used for internode communication between P1 and P5.

Modeling the performance of the hybrid program requires modeling its computation and communication. We can use the performance model for OpenMP applications discussed in Section 3.1 to model the OpenMP performance of the hybrid

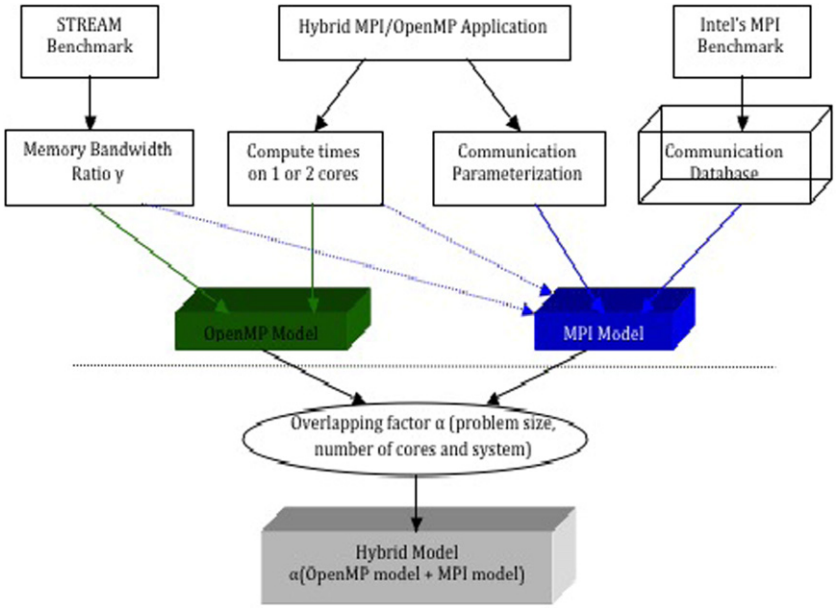

Fig. 4. Framework for modeling hybrid MPI/OpenMP applications.

program. To model the communication of the hybrid program, we just consider internode MPI communication cost. The intranode communication cost (caused by OpenMP directives) is already included in the performance model for OpenMP applications as discussed in Section 3.1. If there is no overlapping between computation and communication in the hybrid program, we just simply sum the performance models of computation and communication to form the performance model of the whole program. Otherwise, we need to consider the overlapping factor for computation and communication.

For the given problem size, number of cores, and system, we define that the factor α for overlapping computation and communication within the hybrid program is

$$\alpha = \frac{\textit{Total Execution Time}}{\textit{Computation Time} + \textit{Communication Time}} \tag{6}$$

The overlapping factor α reflects the overlapping rate between the computation and communication within a hybrid program, and it is associated with the problem size, number of cores and system used. To compute the overlapping factor, we need three measurements for the total execution time, the computation time and communication time on a given number of cores. Then we use least square fit to generate a model for the overlapping factor based on the number of cores to predict the overlapping factor on larger number of cores.

Assume that T_{omp}, T_{mpi} represent the performance models for intranode OpenMP performance and internode MPI communication cost, respectively. When we take the overlapping factor α into account, we have the performance model T of the hybrid program

$$T = \alpha(T_{omp} + T_{mpi}) \tag{7}$$

Then, we can use the performance model to predict the performance of the hybrid program on larger number of cores.

To illustrate the modeling process of a hybrid program discussed above, we present a framework for modeling hybrid MPI/OpenMP applications shown in Fig. 4. Modeling OpenMP or MPI applications discussed in the previous section (Section 3.1) is considered as a special case of the framework above the horizontally dashed line shown in Fig. 4. Modeling an OpenMP-only program requires two components with solid arrows (green in the web version) (i.e., memory bandwidth ratio and computation time); modeling an MPI-only program needs four components with dashed arrows (blue in the web version) (i.e., memory bandwidth ratio, computation time, communication parameterization model and Communication database). Note that, to model a hybrid MPI/OpenMP program, MPI model in Fig. 4 means only MPI communication parameterization model (with Communication database), because OpenMP model includes all computation components and memory bandwidth ratio.

For example, for the given hybrid MPI/OpenMP GTC shown in Section 4, because the workload per core remains the same (weak scaling), the model T_{omp} can be generated by using the modeling method from Section 3.1. Because there are few (only 12) MPI subroutines such as MPI_Sendrecv, MPI_Allreduce, MPI_Reduce, MPI_Allgather, MPI_ Gather, MPI_Bcast, MPI _Send, MPI_Recv, MPI_Comm_size, MPI_Comm_ rank, MPI_Init and MPI _Finalize in the GTC code (note that this is a general case for an MPI program), we can parameterize the MPI communications based on these subroutines as follows. For a given number of cores, MPI_Init and MPI_Finalize can only be called once in an MPI program, so we can manually count

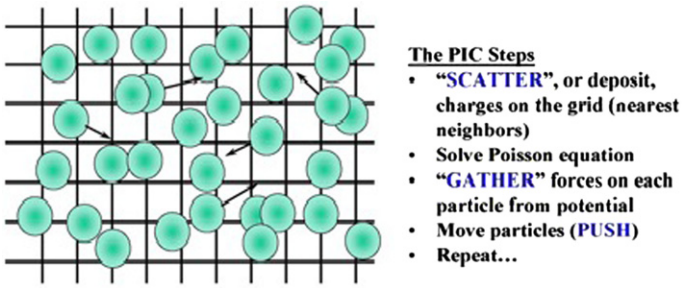

Fig. 5. Particles in cell (PIC) steps [7].

Table 5
Datasets with scaling the number of cores.

Number of cores	4	8	16	32	64	128	256	512
micell	100	100	100	100	100	200	400	800
mecell	100	100	100	100	100	200	400	800
mzetamax	4	8	16	32	64	64	64	64
npartdom	1	1	1	1	1	2	4	8

how many calls and how big the message size for each MPI subroutine to form a communication parameterization model. Generally, this is a straightforward method to generate a parameterization model for the communication cost of an MPI application. We also use the popular Intel's MPI benchmark [9] to measure the performance of each MPI subroutine with different message sizes on different number of cores on each multicore supercomputer, and store the performance data to the Communication database shown in Fig. 4. This kind of measurement just is done once for each supercomputer. Finally, we use the communication parameterization model to estimate the total communication cost based on the performance data from the Communication database.

4. Case study: a hybrid MPI/OpenMP scientific application GTC

In this section, we use the hybrid GTC to validate our performance models on the multicore supercomputers.

4.1. Descriptions of hybrid GTC

GTC [7] is a 3D particle-in-cell application developed at the Princeton Plasma Physics Laboratory to study turbulent transport in magnetic fusion. Fig. 5 presents the basic steps in the GTC code. GTC is currently the flagship SciDAC fusion microturbulence code written in Frotran90, MPI and OpenMP.

The test case for GTC studied in this paper is 100 particles per cell and 100 time steps. The problem sizes for the GTC code are listed in Table 5, where micell is the number of ions per grid cell, mecell is the number of electrons per grid cell, mzetamax is the total number of toroidal grid points, and npartdom is the number of particle domain partitions per toroidal domain.

4.2. Performance model validation

In this section, we use the scientific application GTC (MPI/OpenMP) to validate our performance model for the MPI/OpenMP version of the application on the multicore supercomputers, and use the performance model to calculate and compare the memory bandwidth contention times for the MPI/OpenMP application on three multicore supercomputers: Hydra, P655 and BlueGene/P. Note that, the workload per processor (or core) remains the same for GTC.

4.2.1. OpenMP applications

To illustrate how to use the performance model in Section 3.1, we start to use OpenMP GTC to validate our performance model on Hydra, P655 and BlueGene/P. We use P655 as an example to illustrate how to generate a performance model in detail as follows:

We use the OpenMP STREAM memory benchmark to measure sustainable memory bandwidths for 2 to 8 threads on a compute node on P655, and use the memory bandwidth for 2 threads as a baseline to calculate the bandwidth ratio γ shown in Table 6. We assume the time spent in the computation component per core is T_C, and the time spent in memory bandwidth contention is T_M for 2 threads. (Note that comparing to T_M, the OpenMP overhead for forking and joining the threads is very small.) Then, we have

$$T_2 = T_C + T_M = 1103.37 \tag{8}$$

Table 6
Predicted and actual performance of OpenMP GTC on P655.

Metrics	2 threads	4 threads	8 threads
Actual execution time (s)	1103.37	1202.70	1246.04
Memory bandwidth ratio γ	1 (baseline)	1.75	2.29
Predicted time (s)	Baseline	Baseline	1274.22
Predicted error rate	–	–	2.26%
T_C	970.93		
T_M	132.44		

Table 7
Predicted and actual performance of OpenMP GTC on Hydra.

Metrics	2 threads	4 threads	8 threads	16 threads
Actual execution time (s)	917.91	980.9	1022.83	1153.07
Memory bandwidth ratio γ	1 (baseline)	3.41	7.52	9.21
Predicted execution time (s)	Baseline	Baseline	1088.34	1132.52
Predicted error rate	–	–	6.40%	1.70%
T_C	891.77			
T_M	26.14			

Table 8
Predicted and actual performance of OpenMP GTC on BlueGene/P.

Metrics	2 threads	4 threads
Actual execution time (s)	3279.74	3631.99
Memory bandwidth ratio γ	1 (baseline)	1.98
Predicted execution time (s)	Baseline	Baseline
Predicted error rate	–	–
T_C	2920.30	
T_M	359.44	

Because the workload per core remains the same for GTC, like Eq. (3), we have the following equation for 4 threads

$$T_4 = T_C + 1.75 * T_M = 1202.70 \tag{9}$$

From Eqs. (8) and (9), we have

$$T_C = 132.44 \quad \text{and} \quad T_M = 970.93$$

From Eq. (5), we can predict the performance T_8 for 8 threads as follows:

$$T_8 = T_C + 2.29 * T_M = 970.93 + 2.29 * 132.44 = 1274.22 \text{ (s)}$$

As shown in Table 6, the predicted error rate is only 2.26% for 8 threads. The predicted error rate is the absolute value, and is calculated from the equation (predicted execution time − actual execution time)/(actual execution time). The same method is also applied to other multicore supercomputers shown in Tables 7 and 8. Table 7 shows that the predicted error rate is less than 6.5% for predicting the performance on 8 and 16 threads. It is interesting to see that Hydra has the smallest memory bandwidth contention time, and BlueGene/P has the largest memory contention time for OpenMP GTC because Hydra has the highest memory bandwidth as shown in Table 3, and BlueGene/P has the lowest memory bandwidth as shown in Table 4.

4.2.2. MPI applications

Similarly, in this section, we use MPI GTC to test our performance model on Hydra, P655 and BlueGene/P. For P655, Table 2 shows the sustainable memory bandwidths using MPI STREAM benchmark. We use the memory bandwidth for 8 nodes with 1 core per node as a baseline to calculate the bandwidth ratio γ shown in Table 9.

As shown in Table 9, the predicted error rate is only 1.05% for the 2×4. We can also use the performance model to predict the performance for the 1×8 is 1132.38 seconds, and its predicted error rate is just 1.99%. The same method is applied to other multicore supercomputers as showed in Table 10. The memory bandwidth ratio γ in Table 10 is calculated from Table 3 respectively.

Table 10 shows that the predicted error rate is 4.7% for predicting the performance for the 1×16. The difficulty for our model to deal with is the same memory bandwidth for the 16×1, 8×2 and 4×4 although their execution times are a little bit different. We just pick the execution time for the 16×1 as a baseline. This case also happens on BlueGene/P shown in Table 4. Thus, we will need to consider other factors for our performance model to deal with this case in the future work.

Table 9
Predicted and actual performance of MPI GTC on 8 cores on P655.

Configuration	1 × 8	2 × 4	4 × 2	8 × 1
Actual computation time (s)	1155.38	1133.15	1110.18	1099.08
Memory bandwidth ratio γ	2.50	2.00	1.50	1 (baseline)
Predicted computation time (s)	1132.38	1121.28	Baseline	Baseline
Predicted error rate	1.99%	1.05%	–	–
T_C	1076.88			
T_M	22.2			

Table 10
Predicted and actual performance of MPI GTC on 16 cores on Hydra.

Configuration	1 × 16	2 × 8	4 × 4	8 × 2	16 × 1
Actual computation time (s)	981.62	967.99	944.80	940.02	938.10
Memory bandwidth ratio γ	2.5	1.5	1	1	1 (baseline)
Predicted computation time (s)	1027.77	Baseline	–	–	Baseline
Predicted error rate	4.70%	–	–	–	–
T_C	878.32				
T_M	59.78				

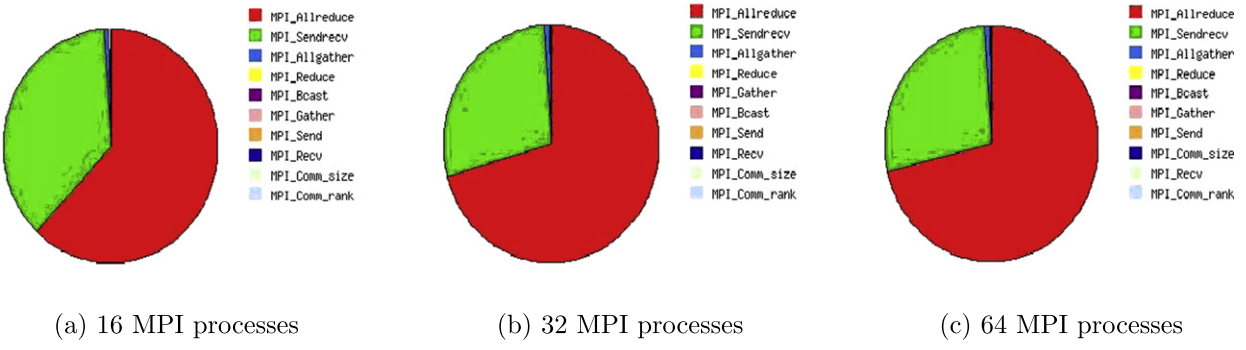

Fig. 6. Communication percentage of each MPI subroutine for hybrid GTC on P655.

Compare Table 9 with Table 6, on P655, we find that the baseline memory bandwidth contention time for MPI GTC is almost six times smaller than that for OpenMP GTC because of OpenMP overhead due to thread creation and increased memory bandwidth contention, however, the pure CPU computation time for MPI GTC is larger than that for OpenMP GTC. Compare Table 10 with Table 7, on Hydra, the baseline memory bandwidth contention time for MPI GTC is over two times larger than that for OpenMP GTC. This is consistent with Table 3 where the sustainable memory bandwidth for using 16 OpenMP threads is larger than that for using 16 MPI processes per node.

4.2.3. Hybrid MPI/OpenMP applications

In this section, we apply our performance modeling framework proposed in Fig. 4 to model the performance of the hybrid MPI/OpenMP GTC on the three multicore supercomputers.

In Section 4.2.1, we discussed the OpenMP models for the OpenMP GTC on the three supercomputers. We use the OpenMP models to model the performance of the hybrid GTC because the hybrid GTC is a weak-scaling application. Now we mainly focus on generating a parameterized communication model for the hybrid GTC. As we discussed in Section 3.2, there are few (only 12) MPI subroutines such as MPI_Sendrecv, MPI_ Allreduce, MPI_Reduce, MPI_ Allgather, MPI_Gather, MPI_Bcast, MPI_ Send, MPI_Recv, MPI_Comm _size, MPI_Comm_rank, MPI_Init and MPI_ Finalize in the GTC code. We use IPM [10] to collect MPI communication performance and its profiling (message size and number of calls). We observe that the MPI subroutines MPI_Allreduce, MPI_ Sendrecv and MPI_Allgather dominate more than 98% of the total communication time shown in Fig. 6, which shows the communication percentage of each MPI subroutine for the hybrid GTC on P655.

Tables 11, 12 and 13 show the main MPI profilings of the hybrid GTC for 16, 32 and 64 MPI processes. MPI_ Allreduce with four different message sizes is performed for each program execution across Tables 11, 12 and 13, however, the number of calls for MPI_Allreduce is double with doubling the number of MPI processes. Similarly, MPI_Sendrecv with two different message sizes is performed for each program execution across Tables 11, 12 and 13, however, the number of calls for MPI_Sendrecv is doubled with doubling the number of MPI processes. For MPI_Allgather, the message size decreases by half and the number of calls is doubled with doubling the number of MPI processes because of the fixed total message size (array size). Based on the communication characteristics of the hybrid GTC from IPM, we can manually parameterize the

Table 11
Main MPI profiling of GTC for 16 MPI processes.

16 processes	Message size (bytes)	Number of calls
MPI_Allreduce	4	3200
MPI_Allreduce	364	3600
MPI_Allreduce	1168164	3200
MPI_Allreduce	20	1600
MPI_Sendrecv	129796	28800
MPI_Sendrecv	8	6400
MPI_Allgather	519184	3200

Table 12
Main MPI profiling for 32 MPI processes.

32 processes	Message size (bytes)	Number of calls
MPI_Allreduce	4	6400
MPI_Allreduce	364	7200
MPI_Allreduce	1168164	6400
MPI_Allreduce	20	3200
MPI_Sendrecv	129796	57600
MPI_Sendrecv	8	12800
MPI_Allgather	259592	6400

Table 13
Main MPI profiling for 64 MPI processes.

64 processes	Message size (bytes)	Number of calls
MPI_Allreduce	4	12800
MPI_Allreduce	364	14400
MPI_Allreduce	1168164	12800
MPI_Allreduce	20	6400
MPI_Sendrecv	129796	115200
MPI_Sendrecv	8	25600
MPI_Allgather	129796	12800

Table 14
Predicted performance of hybrid GTC on P655.

Number of cores	8	16	32	64	128	256	512
Actual runtime (s)	1246.04	1306.89	1363.96	1370.24	1388.23	1347.04	1424.53
Prediction (s)	1274.22	1280.15	1288.00	1301.71	1332.41	1397.19	1461.03
Error (%)	2.26%	2.05%	5.57%	5.00%	4.02%	3.72%	2.56%

communication time for each MPI subroutine by the product of the time for each MPI subroutine with the given message size and number of processors and the number of calls to build the parameterized communication model.

For internode communication, we use Intel's MPI benchmarks (IMB) to measure the performance for each MPI subroutine with different message sizes on different number of cores, then store them to the Communication database. For each MPI subroutine, we query the Communication database to get the communication time for a message size on a given number of nodes, then use the product of the time and the number of calls for the subroutine to calculate its total communication time. Based on the performance data for IMB from the Communication database, we can use the parameterized communication model to calculate the total communication time.

Because of the use of blocking communications in the entire GTC, we observe that the overlapping factor for computation and communication is almost 1, so we use the factor to generate our performance model for GTC. In the following, we present the experimental results for our performance models to predict the performance of the hybrid GTC on P655, Hydra and BlueGene/P.

Table 14 shows the predicted performance of hybrid GTC using our performance model on P655. Because the workload per core remains the same for GTC (weak scaling), we use the OpenMP model for OpenMP GTC on 8 cores as baseline, then sum the baseline OpenMP performance and total MPI communication time to predict the performance of the hybrid GTC. The error rate is less than 5.58%.

Table 15 shows the predicted performance of hybrid GTC using our performance model on Hydra. We use the OpenMP model for OpenMP GTC on 16 cores as baseline, then sum the baseline OpenMP performance and total MPI communication time to predict the performance of the hybrid GTC. The error rate is less than 7.77%.

Table 15
Predicted performance of hybrid GTC on Hydra.

Number of cores	16	32	64	128	256	512
Actual runtime (s)	1153.07	1200.66	1239.26	1225.91	1210.45	1190.5
Prediction (s)	1132.52	1137.27	1143.07	1154.66	1175.10	1230.03
Error (%)	1.70%	5.28%	7.76%	5.81%	2.92%	3.32%

Table 16
Predicted performance of hybrid GTC on BlueGene/P.

Number of cores	4	8	16	32	64	128	256	512
Actual runtime (s)	3631.99	3681.05	3716.67	3738.52	3771.67	3761.81	3741.22	3742.49
Prediction (s)	–	3644.98	3659.62	3685.78	3707.14	3794.42	3927.34	3906.22
Error (%)	–	0.98%	1.54%	1.41%	1.71%	0.87%	4.97%	4.37%

Table 16 shows the predicted performance of hybrid GTC using our performance model on BlueGene/P. We use the OpenMP model for OpenMP GTC on 4 cores as baseline, then sum the baseline OpenMP performance and total MPI communication time to predict the performance of the hybrid GTC. The error rate is less than 4.98%.

In summary, we apply our performance modeling framework to weak-scaling hybrid applications to model and predict the performance of the hybrid GTC on up to 512 cores on P655, Hydra and BlueGene/P with less than 7.77% error rate. This indicates that our modeling method is accurate and practical.

5. Related work

Levesque et al. [11] observed that the primary source of contention when moving from single core to dual core on AMD Opteron architecture is memory bandwidth, and proposed a simple performance model for sequential applications to extrapolate the quad-core performance by assuming the time spent in the execution component remains the same, but the time spent in memory bandwidth contention will increase proportional to the reduction in effective memory bandwidth per core. In this paper, we generalize the performance model for OpenMP and hybrid parallel applications to extrapolate the performance of the multicore node (which consists of one or several multicores).

Barker et al. [5] discussed using performance modeling to design large scale systems throughout their life cycle from early design through production use, presented an application-centric performance model development framework, and addressed the importance of performance modeling. Our performance model has more focus on multicore, and takes into account memory bandwidth contention from multicore.

Adhianto and Chapman [1] proposed a cost efficient approach to model and evaluate parallel OpenMP, MPI and hybrid MPI + OpenMP with reasonable accuracy based on a combination of static analysis (using the OpenUH compiler) and feedback from runtime benchmarks (Sphinx and Perfsuite) for both communication and multithreading efficiency measurement, and predicted the performance of a parallel matrix multiply using Cannon algorithm.

Aversa et al. [4] described simulation-based techniques for performance prediction of hybrid MPI/OpenMP code in different working conditions using HeSSE (Heterogeneous System Simulation Environment), and predicted the performance of a parallel N-body code on an SMP cluster.

There are many approaches to modeling MPI communication cost, such as LogP [6], LogGP [2], collective communication models [21] and so on, in this paper, we just take a straightforward empirical method to manually parameterize the communication time for each MPI subroutine by the product of the time for each MPI subroutine with the given message size and number of processors, and the number of calls on the given system to generate a parameterized communication model, then based on the performance data for each MPI subroutine on a given system stored in the Communication database, we can estimate the total communication cost on the system.

6. Conclusions

In this paper, we analyzed and compared the performance of MPI, OpenMP and hybrid applications on three large-scale multicore supercomputers, IBM POWER4, POWER5+ and BlueGene/P using MPI and OpenMP STREAM benchmarks, Intel's MPI benchmarks and the hybrid MPI/OpenMP GTC, and presented a practical performance modeling framework for weak-scaling hybrid MPI/OpenMP applications based on the memory bandwidth contention time and the parameterized communication model to model and predict the performance of hybrid and OpenMP GTC on these multicore supercomputers. The experimental results for our performance modeling method showed less than 7.77% error rate in predicting the performance of the hybrid MPI/OpenMP GTC on up to 512 cores on the three multicore supercomputers. We also used the performance model to estimate and compare the memory bandwidth contention times for the MPI and OpenMP GTC.

For weak-scaling scientific applications, the measured sustained memory bandwidth can provide insight into the memory bandwidth that a system should sustain on these scientific applications with the same amount of workload per core. However, for strong scaling scientific applications, it is hard to measure the sustained memory bandwidth for the different

amount of decreased workload per core. This is a limitation for our performance modeling framework. We believe that our performance modeling framework can be applied to any weak-scaling hybrid MPI/OpenMP applications with memory bandwidth contention problems. Our future work will focus on exploring performance modeling for strong scaling scientific applications, and investigating performance-power trade-off models in our MuMMI project [13].

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